Overview of Developments in MANTID relating to Indirect Inelastic Spectroscopy July 2017 - June 2018

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Overview of Developments in MANTID relating to Indirect Inelastic Spectroscopy July 2017 - June 2018

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Abstract

The Manipulation and Analysis Toolkit for Instrument Data (MANTID) is an open source crossplatform application that provides a framework for data reduction and analysis relating to neutron and muon techniques.

This report provides an outline of the developments to the Indirect Inelastic neutron spectroscopy routines, within MANTID between the months of July 2017 and June 2018 including Mantid release 3.11-3.13. Notable changes include the addition of Monte-Carlo routines for QENS absorption corrections and error propagation in $I(Q,t)$. The QENS fitting interfaces have been extended to allow for defining custom ties and constraints as well as fitting across multiple datasets.

Contents

Acknowledgements

1 Introduction

The MANTID project is a cross platform, open source framework which supports the manipulation of scientific data [1]. The software is designed to reduce, analyse and visualise data from neutron scattering and muon spectroscopy research facilities across the globe.

There have been contributions to the development of this framework from Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, US, the ISIS Muon and Neutron Source based at Rutherford Appleton Laboratory, UK, and the Institut Laue-Langevin (ILL), France, and the currently under construction European Spallation Source (ESS), Sweden.

The majority of the MANTID project is written in C++ and Python. The framework can be accessed through a graphical user interface (GUI) or through a user script. The workflow consists of using several predefined algorithms which manipulate data stored in workspaces, typically experimental data recorded by detectors and monitors. A workspace within MANTID is a structure containing x, y and error data. The MANTID framework also provides data visualisation and graphing tools.

This report details the addition of Monte-Carlo algorithms for calculating absorption corrections for quasi-elastic neutron scattering (QENS) data and for error-propagation in the intermediate scattering function, $I(Q,t)$. Also outlined are the significant changes made to the routines and interfaces for fitting QENS data in MANTID [2, 3, 4, 5]. This report outlines the addition of custom ties, constraints, user-defined functions and multiple dataset fitting to the QENS fitting interfaces. In addition, this report covers developments relating to indirect diffraction and the Vesuvio instrument.

2 Model-View-Presenter

Model-view-presenter is an architectural software pattern used in the design of user interfaces. The model-view-presenter pattern facilitates automated unit test as well as decoupling of the business logic, presentation logic and the graphical interface. The 'model' is an interface which outlines the accessible data and transformations. The 'view' defines how data is to be displayed and passes user events to the presenter. The 'presenter' mediates between the view and model; user events from the view are used to update the model and data from the model is formatted to be displayed in the view. Figure 1 visually depicts the model-view-presenter pattern.

Restructuring the indirect inelastic interfaces to meet the requirements of the model-view-presenter pattern is an ongoing development task within MANTID. As of MANTID version 3.13, the QENS fitting interfaces have been redesigned to follow the requirements.
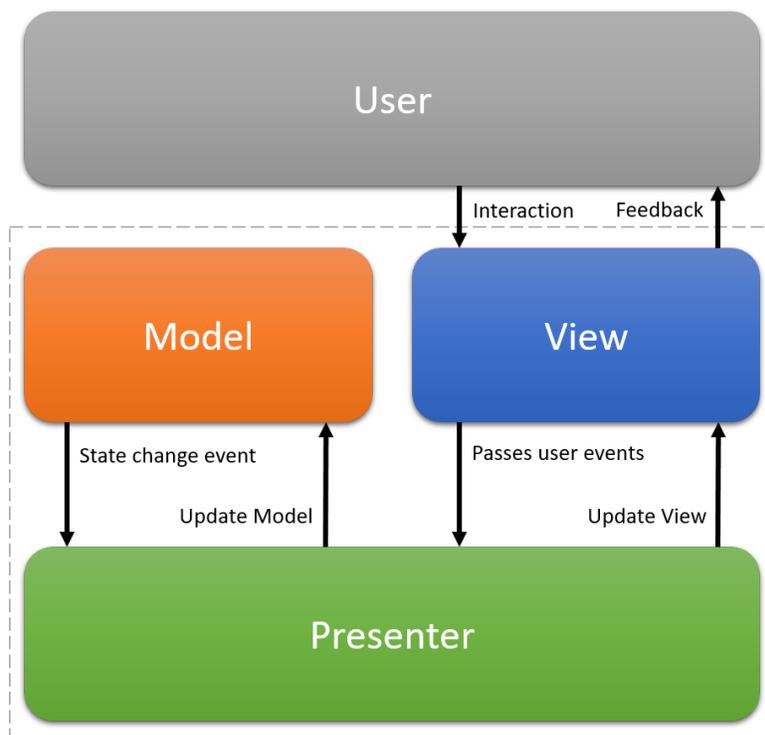
Figure 1: A visual depiction of the model-view-presenter pattern

3 Data Reduction

Either a Python script or the custom user interfaces can be used to reduce indirect neutron spectroscopy data in MANTID. The 'Energy Transfer' interface (Figure 2) is used to convert the raw time-of-flight experiment data into energy transfer. Options for grouping detectors and rebinning data are available. A calibration and resolution workspace, for use in indirect data reduction and analysis, can be created using the 'Calibration' interface. The dynamic structure factor can be calculated using the '$S(Q, \omega)$' interface.
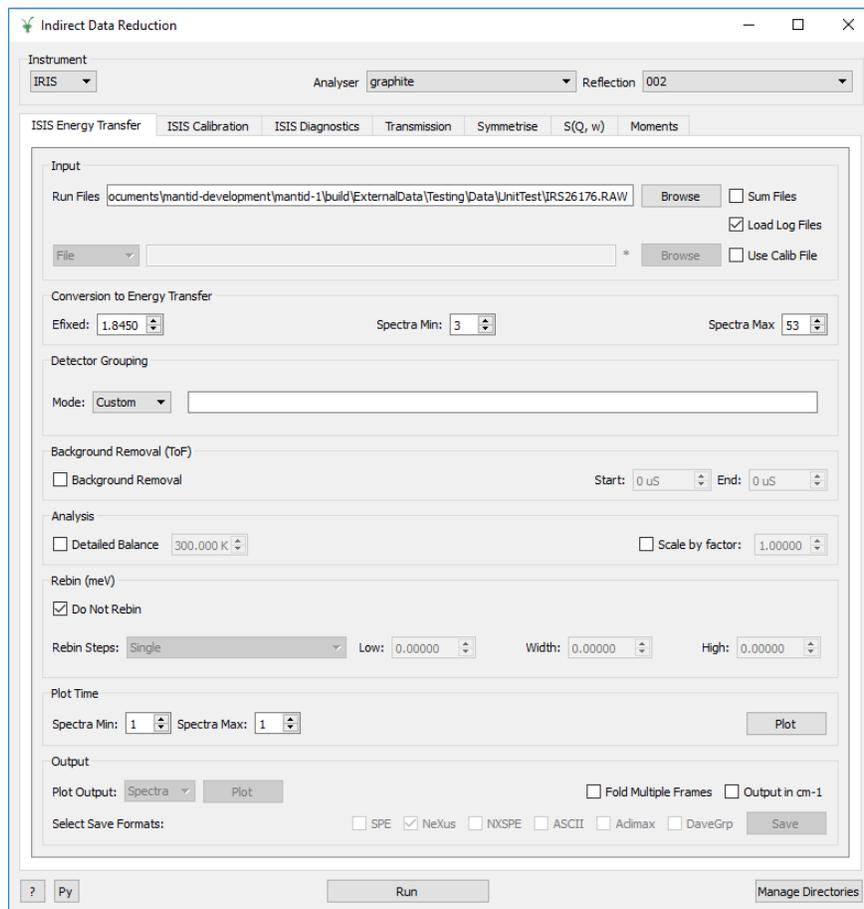
Figure 2: The ISIS Energy Transfer interface; used for reducing raw time-of-flight data (at the ISIS neutron facility) to energy transfer

Version 3.13 of MANTID introduced a 'Custom' option under 'Detector Grouping' in the 'Energy Transfer' interface, as shown in Figure 3. The 'Custom' option provides a text field in which specific detector ranges may be selected for grouping. A range of detectors to be grouped can be specified using the format 'A-B', where 'A' is the first detector in the group and 'B' is the final detector. Groups must be separated by a comma.

Figure 3: The Detector Grouping section of the ISIS Energy Transfer interface; the 'Custom' option has been selected

4 QENS Corrections

4.1 Paalman-Pings method for absorption corrections

Corrections for reduced QENS (quasi-elastic neutron scattering) data are applied in MANTID using the numerical evaluation method outlined by Paalman and Pings [6]. The Paalman-Pings method for applying absorption corrections involves the absorption factors outlined in Table 1.

Symbol	Scatter From	Absorbed By
$A_{s,s}$	Sample	Sample
$A_{s,sc}$	Sample	Sample, Container
$A_{c,c}$	Container	Container
$A_{c,sc}$	Container	Sample, Container

Table 1: Description of the Paalman-Pings absorption factors

The application of the absorption factors using the Paalman-Pings method is as follows:

$$I_s = \frac{1}{A_{s,sc}} \left(I_{sc}^E - K_c I_c^E \frac{A_{c,sc}}{A_{cc}} \right) \tag{1}$$

where I_s is the corrected sample data, K_c is the container scale factor, I_{sc}^E is the sample data before corrections are applied and I_c^E is the container data.

4.2 Monte Carlo method for calculating absorption corrections

The 'MonteCarloAbsorption' algorithm in MANTID can be used to calculate the Paalman-Pings absorption factors using a Monte Carlo approach. The full description of this algorithm is available within the online MANTID user documentation [7].

A new algorithm available in MANTID version 3.11 [8], 'SimpleShapeMonteCarloAbsorption', provides properties for defining the sample and container shapes from one of three possibilites: 'Flat Plate', 'Cylinder' and 'Annulus'. The 'SimpleShapeMonteCarloAbsorption' algorithm will define the geometry on the input data before passing it as input to the 'MonteCarloAbsorption' algorithm.

In addition to the 'SimpleShapeMonteCarloAbsorption' algorithm, an indirect specific Monte Carlo absorption correction algorithm was introduced in MANTID version 3.11, 'CalculateMonteCarloAbsorption'. The 'CalculateMonteCarloAbsorption' algorithm, takes the sample data and the empty container data as inputs and produces two of the four Paalman-Pings absorption factors: $A_{s,s}$ and $A_{c,c}$. As only two of the four factors are calculated by the 'CalculateMonteCarloAbsorption' algorithm, a revision of Equation 1 was required in order to apply the output factors:

$$I_s = \frac{I_{sc}^E}{As, s} - K_c \frac{I_c^E}{A_{c,c}} \tag{2}$$

where I_c^E is the container data, K_c is the container scale factor, $A_{s,s}$ and $A_{c,c}$ are the absorption factors defined in Table 1.

A new interface 'Calculate Monte Carlo Absorption' (depicted in Figure 4) has been added within the 'Indirect Corrections' interfaces in MANTID, as of version 3.11. This interface facilitates the use of the 'CalculateMonteCarloAbsorption algorithm. The 'Apply Absorption Corrections' interface has been modified such that the correct application of the corrections is selected depending on the number of provided absorption factors within the input corrections.
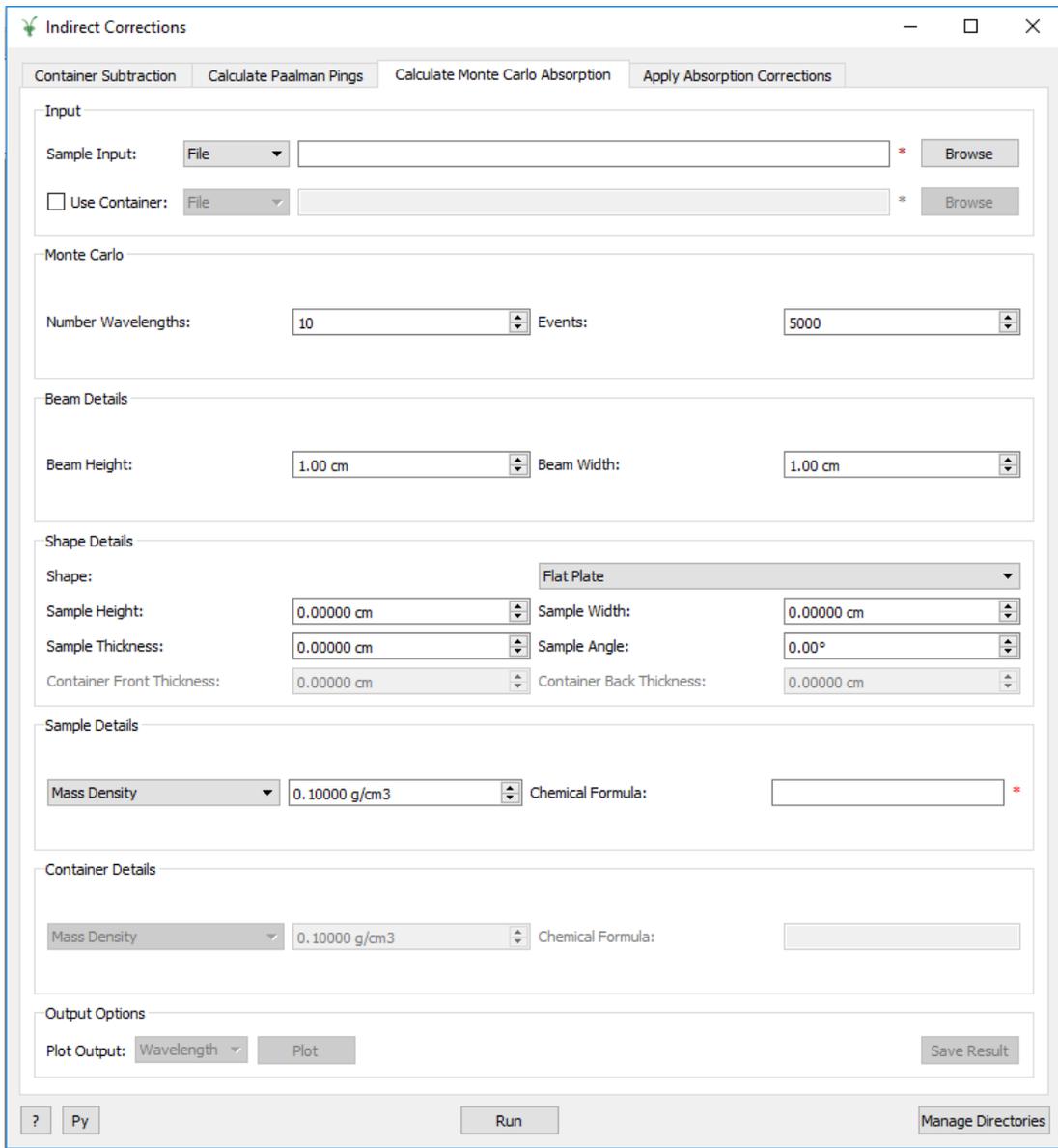
Figure 4: The Calculate Monte Carlo Absorption interface

5 QENS Data Analysis

5.1 Error propagation in I(Q,t)

A Monte-Carlo routine for calculating the errors in I(Q,t) has been introduced in MANTID version 3.13. The error calculation routine has been included in the 'TransformToIqt' algorithm. Two new input properties for modifying the Monte-Carlo routine are available when using 'TransformToIqt': 'NumberOfIterations' and 'SeedValue'.

To calculate errors in $I(Q,t)$, multiple $S(Q,\omega)$ workspaces are generated within experimental error of the input $S(Q,\omega)$. Each of these $S(Q,\omega)$ workspaces is generated using a Mersenne Twister pseudo-random generator. The 'NumberOfIterations' input property defines the number of $S(Q,\omega)$ to be created. The 'SeedValue' input property defines the seed to use in the pseudo-random number generation. $I(Q,t)$ is calculated for each of the generated workspaces and their standard deviation is taken as the error.

The '$I(Q,t)$' interface in MANTID, used for calculating $I(Q,t)$ from $S(Q,\omega)$ provides an option for selecting the number of iterations in the Monte-Carlo error calculation routine, as shown in Figure 5.

5.2 Peters and Yi Models

Additional models for mean-squared displacement fitting were introduced in MANTID version 3.11: Peters model [9] and Yi model [10]. The Peters and Yi models are available in the MANTID library of functions and have been included under the 'Fit Type' drop-down menu in the 'MSDFit' interface.

'Gaussian' is appropriate for isotropic motion in homogeneous materials within harmonic potential. This model doesn't consider vibrational or rotational motion and is generally applicable for low Q values.

'Peters' is appropriate for samples where motion heterogeneity, i.e., distribution of MSD among several atoms in the sample, is present. This model should work for higher values of Q.

'Yi' is appropriate for samples with single atom motion in anharmonic potential as well as when dynamical inhomogeneity arises due to distribution of MSD among several atoms in the sample. This model considers terms up to Q^4, as such it is applicable for large values of Q.
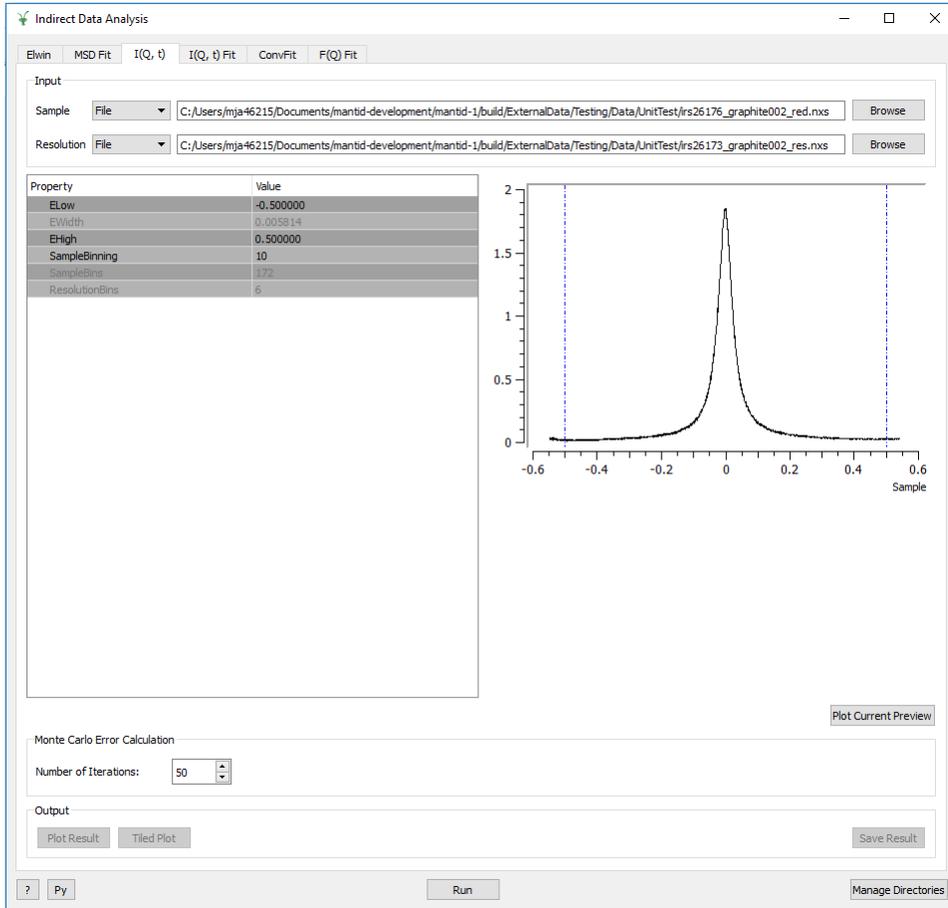
Figure 5: The $I(Q, t)$ interface

5.3   New fitting algorithms

Two new QENS fitting algorithms, 'QENSFitSequential' and 'QENSFit-Simultaneous', were included in MANTID version 3.13. The 'QENSFit-Sequential' and 'QENSFitSimultaneous' algorithms can be used for fitting QENS data sequentially or simultaneously, respectively. Specializations of the QENS fitting algorithms are included for convolution fitting and fitting of $I(Q, t)$: 'ConvolutionFitSequential', 'ConvolutionFitSimultaneous', 'Iqt-FitSequential', 'IqtFitSimultaneous'. The 'MSDFit' and '$F(Q)$ Fit' interfaces have been modified to use the 'QENSFitSequential' algorithm. The '$I(Q, t)$ Fit' and 'ConvFit' interfaces utilise the 'ConvolutionFitSequential'

and 'IqtFitSequential' algorithms, respectively.

An algorithm for extracting individual members of a fit, 'ExtractQENS-Members' was introduced in MANTID version 3.12. The 'ExtractQENS-Members' algorithm generates a MANTID workspace group containing the fit, difference and each fitted function within individual workspaces. The workspaces created by 'ExtractQENSMembers' have x-axis units of 'Q'.
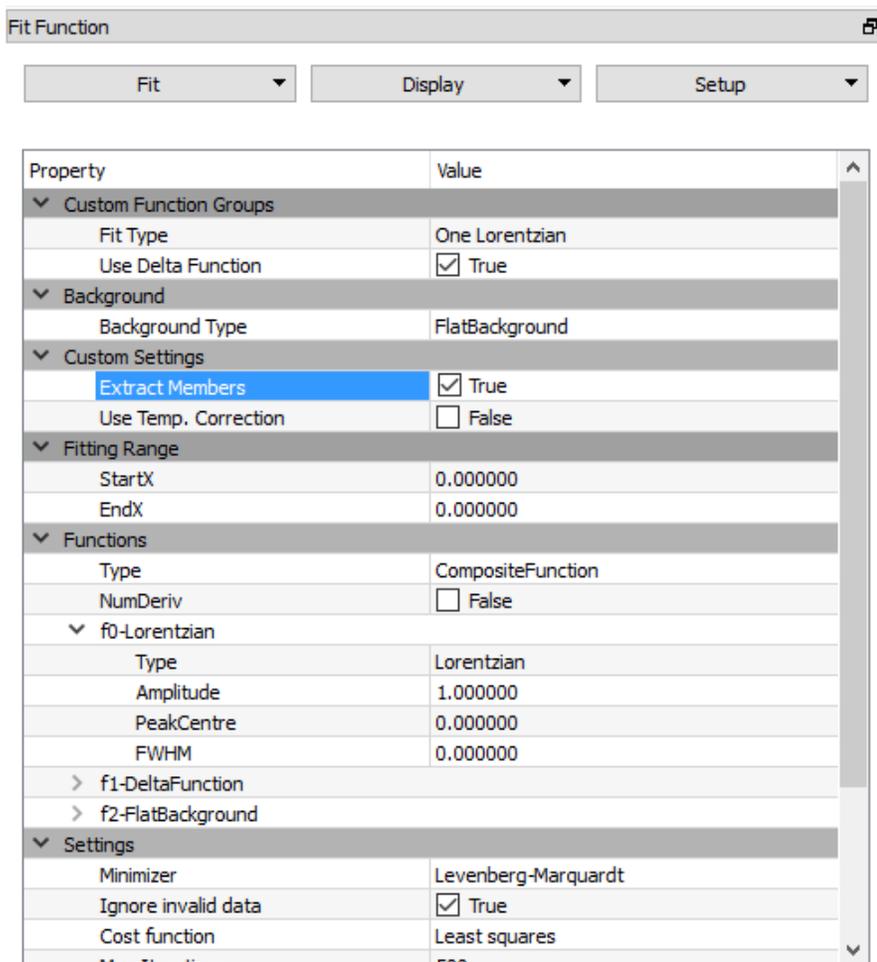
Figure 6: The function browser; used for defining the fit function and settings
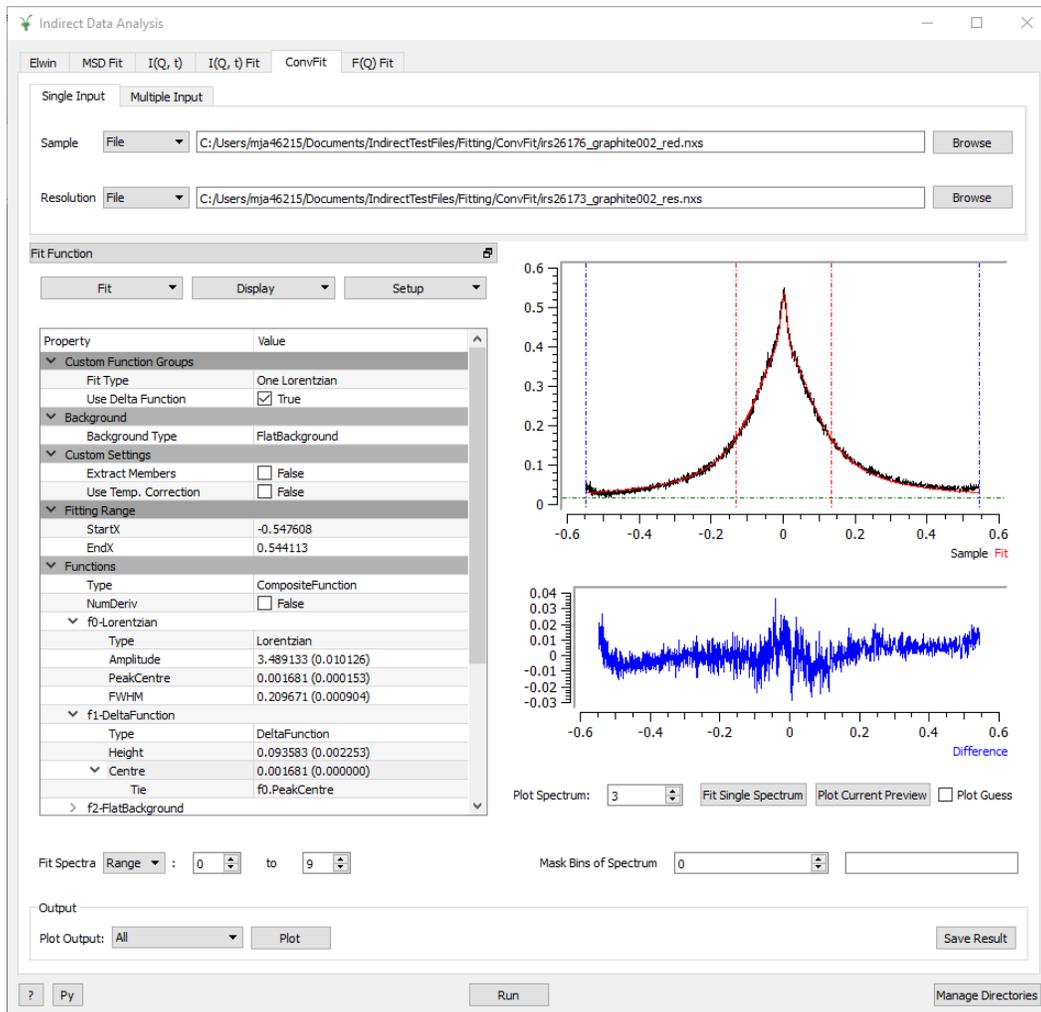
Figure 7: The 'ConvFit' interface in single-input mode

5.4 Interface Layout

As of MANTID version 3.12, the input data and fit result are plot separately from their difference in the QENS fitting interfaces. The difference between the input data and fit result is often sufficiently small such that it cannot be distinguished from the line $y = 0$. The difference plot has been added below the plot of the input data, fit result and guess.

The browsers for defining the fitting function and settings of the fit (e.g.

minimiser, cost function) has been combined into a single browser, depicted in Figure 6, in MANTID version 3.12. Common fitting models can be found for quick access under the 'Custom Function Groups' menu in the browser.

The layout of the 'MSD Fit', '$I(Q, t)$ Fit' and 'ConvFit' interfaces are shown in Figures 8, 9 and 7, respectively.
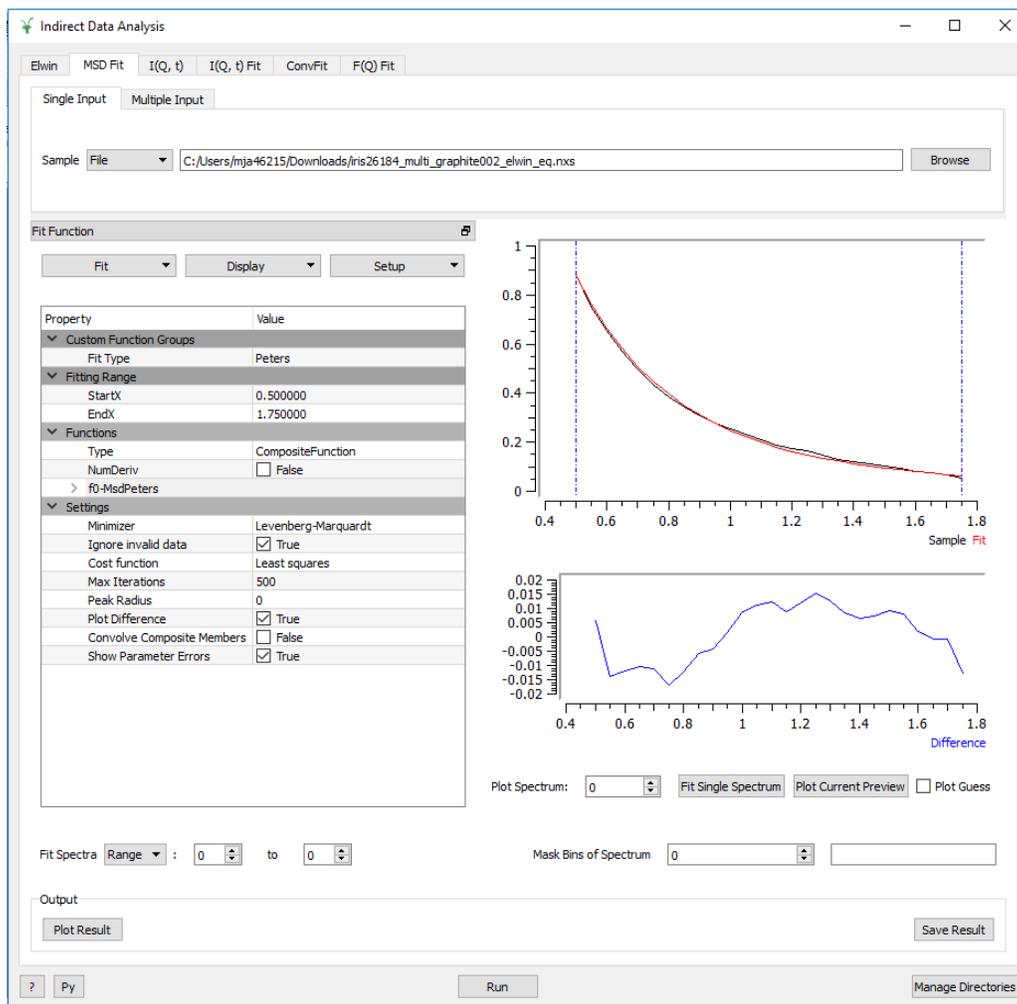
Figure 8: The 'MSD Fit' interface in single-input mode

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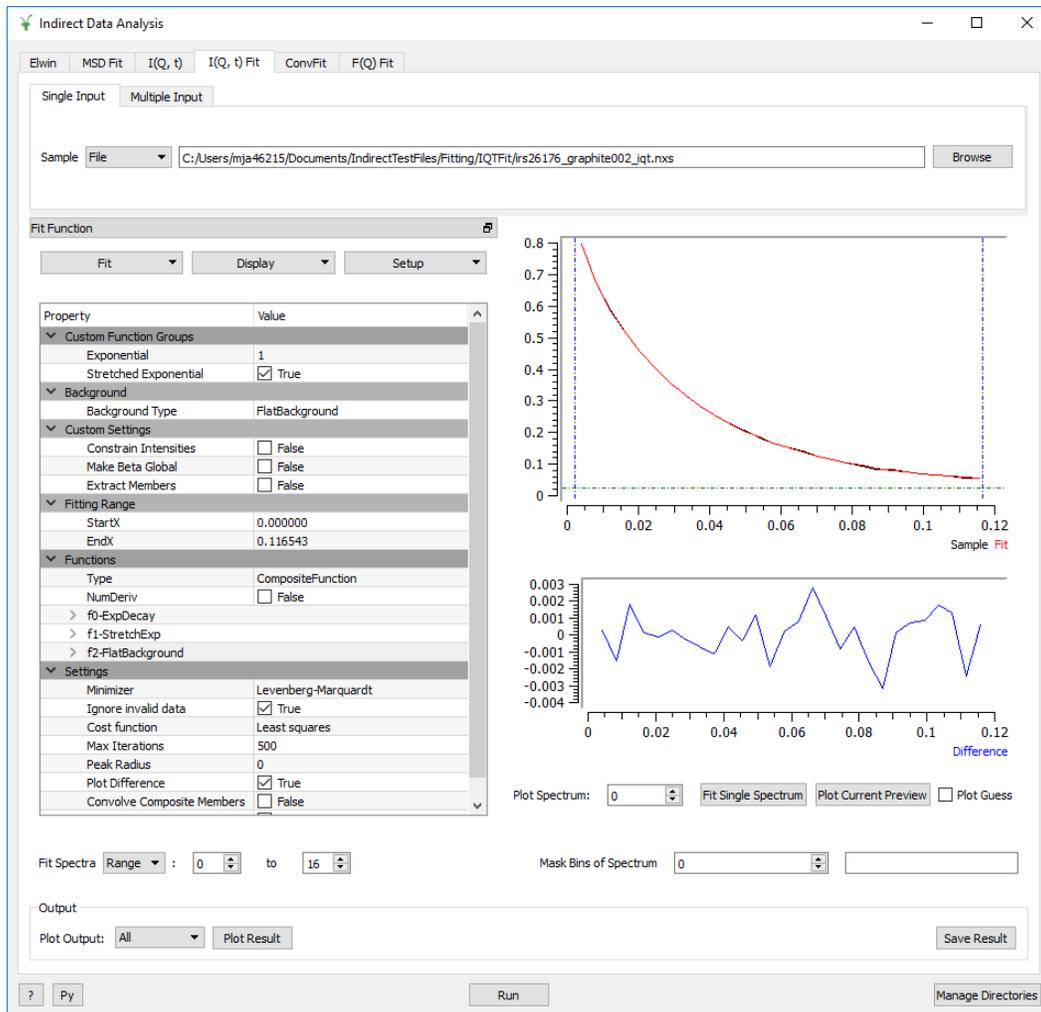
Figure 9: The '$I(Q, t)$ Fit' interface in single-input mode

5.5 F(Q) fitting

The 'JumpFit' interface, available in MANTID version 3.12 and earlier, used for fitting the full-width-half-maximum resulting from a convolution fit, has been modified and renamed to '$F(Q)$ Fit' (see Figure 10). The '$F(Q)$ Fit' interface requires the result of a convolution fit as input and is used to fit a parameter, extracted from the input, across all Q. In addition to the option of fitting the full-width-half-maximum, it is now possible to fit the elastic

incoherent scattering factor (EISF).

The 'Fit Parameter' drop-down menu in the '$F(Q)$ Fit' interface allows for selection of the parameter type to fit; either 'Width' or 'EISF'.The adjacent drop-down menu, labelled with the selected parameter type, can be used to select the specific parameter from the input.
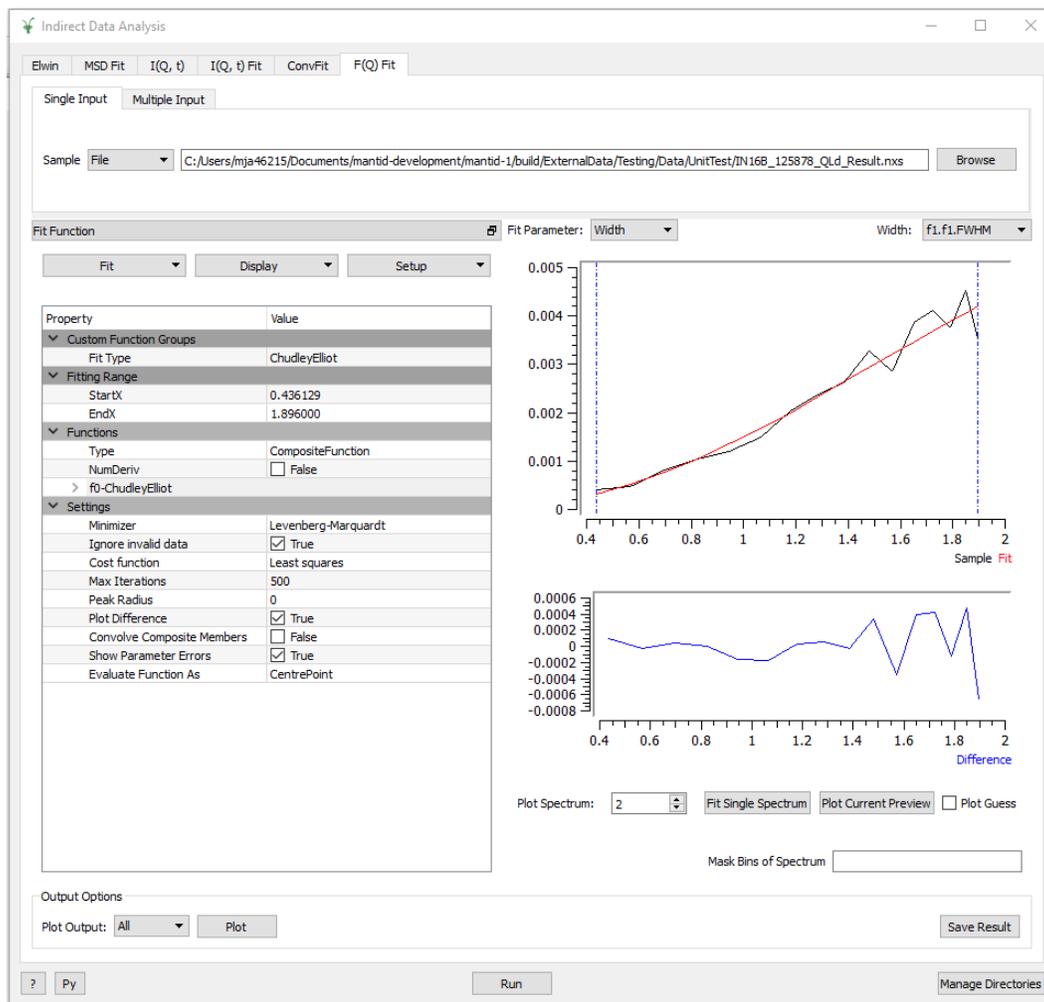
Figure 10: The $F(Q)$ Fit interface in single-input mode

5.6 Custom Ties

Parameters of a fitting function can be tied to mathematical expressions in MANTID; a tie may include other parameters in the function. Custom ties are now available within the QENS fitting interfaces. To add a custom tie to a parameter, the parameter can be right-clicked to bring up a pop-up menu consisting of the options 'Fix', 'Constraint' and 'Tie' (see Figure 11). Hovering the mouse cursor over 'Tie' will bring up a sub-menu with the options 'To function' and 'Custom Tie'. The 'To function' option will provide a drop-down menu of parameters with the same name in different functions. The 'Custom Tie' option provides a text-box in which a mathematical expression may be entered (as depicted in Figure 12).
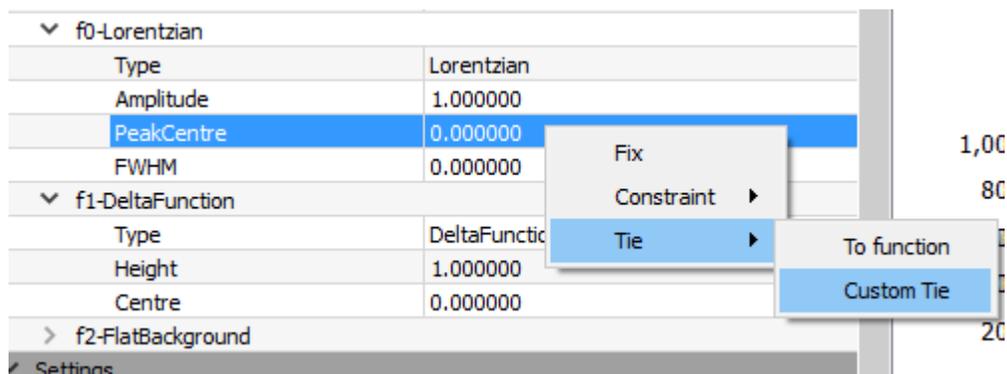
Figure 11: The 'Tie' menu
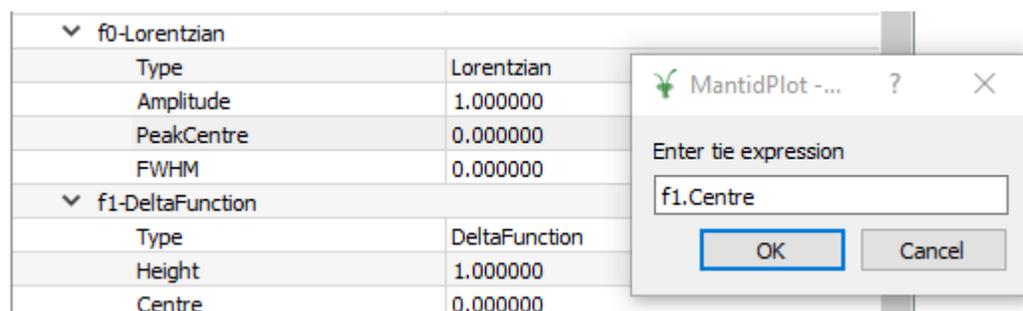
Figure 12: The 'Custom Tie' pop-up menu provides a text field for entering the tie expression

5.7 Constraints

Boundary constraints on parameters can be set within the QENS fitting interfaces, as of MANTID version 3.12. To add a constraint to a parameter, it must be right-clicked within the interface to bring up the menu. Within that menu is the 'Constraint' sub-menu. An upper bound, lower bound or both may be set on the parameters of the fit functions shown in the interfaces (see Figure 13). The constraints are displayed below the parameter and may be modified, as depicted in Figure 14.
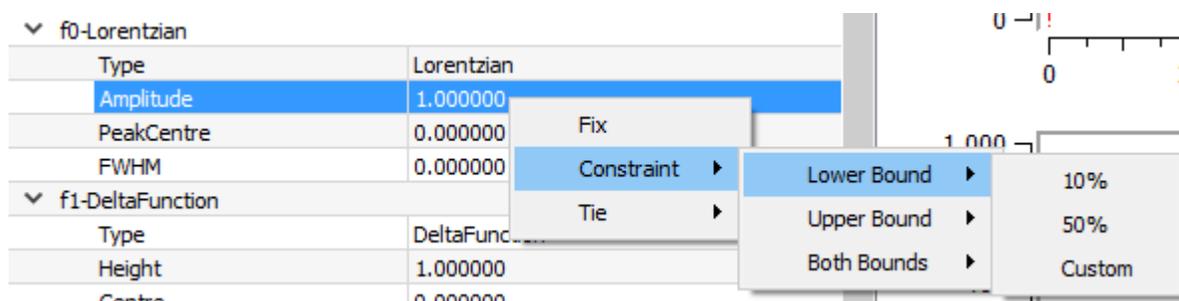
Figure 13: The 'Constraint' menu

Figure 14: A custom constraint on both bounds is shown under the parameter

5.8 User-defined functions

MANTID's library of functions, including custom user-defined functions are now available from within the QENS fitting interfaces, as of version 3.12. All functions can be found by right-clicking on either the 'Functions' menu or the composite in the browser you wish to add the function to and selecting 'Add Function' in the menu. (see Figure 15).
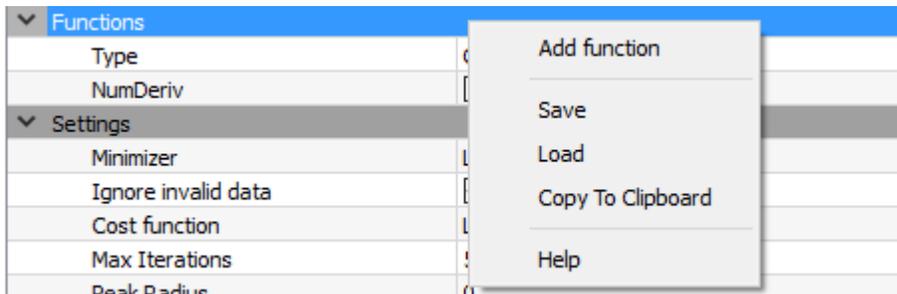
Figure 15: The menu appearing when a composite function or 'Functions' is right-clicked

After clicking 'Add Function', a categorised menu of the available functions will be presented (as shown in Figure 16), selecting the required function and clicking 'Ok' will add it to the model.
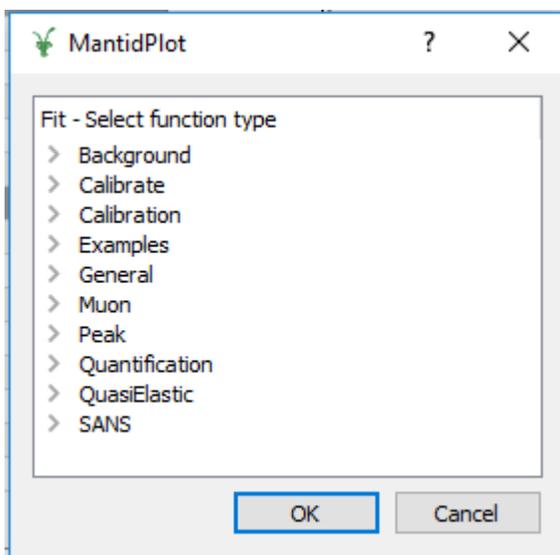
Figure 16: The function selection menu; functions are categorised

5.9 Fitting discontinuous spectra ranges

MANTID version 3.13 introduced the selection of discontinuous spectra ranges within the QENS fitting interfaces. A drop-down menu, labelled 'Fit Spectra' is provided to allow providing either a continuous or discontinuous range

of spectra. If 'Range' is selected, two number fields are provided to select
the minimum and maximum of a continuous spectra range (see Figure 17).
If 'String' is selected, a text field is provided (see Figure 18) in which a dis-
continuous spectra range may be selected. A discontinuous range must be
provided as a comma-separated list of single spectrum or continuous spectra
ranges, defined with the syntax 'A-B' where 'A' and 'B' are integers.
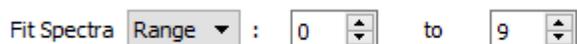
Figure 17: Spectrum range selection in the QENS fitting interfaces, found
below the function

Figure 18: Discontinuous spectra selection in the QENS fitting interfaces,
found below the function

5.10   Masking of energy regions

The masking of energy regions is an available feature within the QENS fitting
interfaces as of MANTID version 3.13. The masking component of the QENS
fitting interfaces is shown in Figure 19 and can be accessed via The drop-
down menu right-adjacent to the 'Mask Bins of Spectrum' label allows a
spectrum to be selected. Once the spectrum to be masked is selected, a
comma separated list of pairs can be provided to define the energy regions
to mask. Each pair defines a region to be masked.

Figure 19: The masking component of the QENS fitting interfaces, found
below the plots

5.11 Multiple dataset fitting

A multiple dataset mode has been added to each of the QENS fitting interfaces, as of MANTID version 3.13. A dataset in MANTID is a single spectrum within a workspace. The QENS fitting interfaces may be switched to multiple dataset mode by clicking the 'Multiple Input' tab at the top of the interface. The multiple dataset mode of the 'MSD Fit', '$I(Q,t)$ Fit', 'ConvFit' and '$F(Q)$ Fit' interfaces is depicted in Figures 20, 21, 22 and 23, respectively.
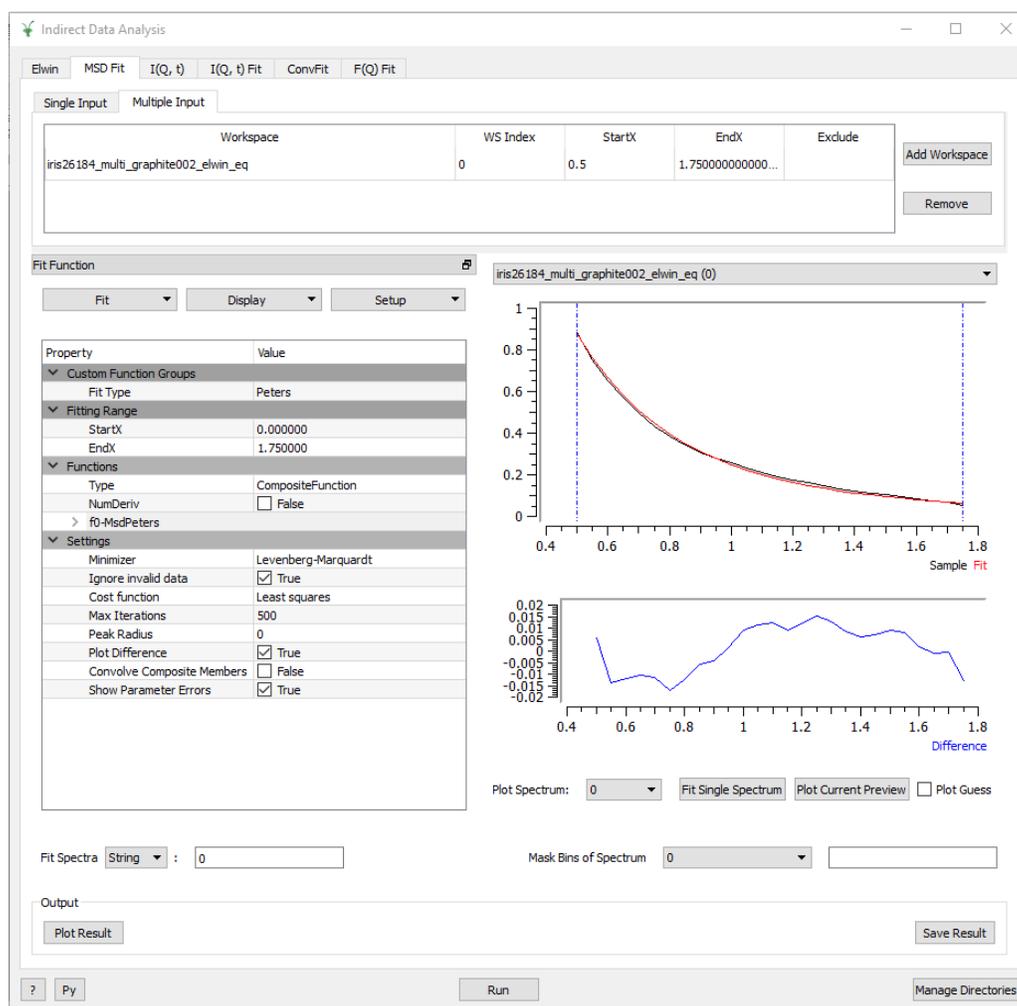
Figure 20: The 'MSD Fit' interface in multiple-input mode
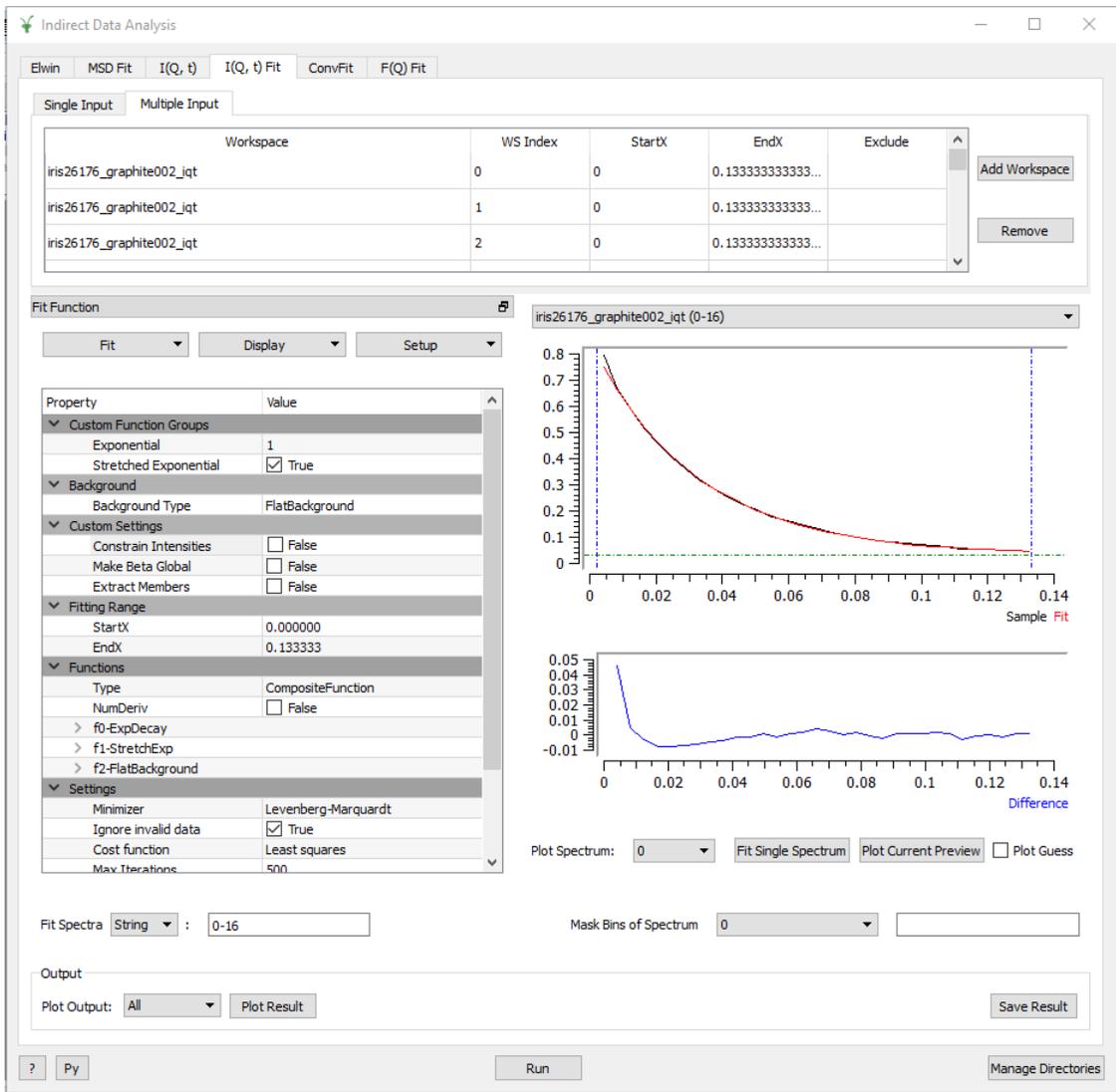
Figure 21: The '$I(Q,t)$Fit' interface in multiple-input mode
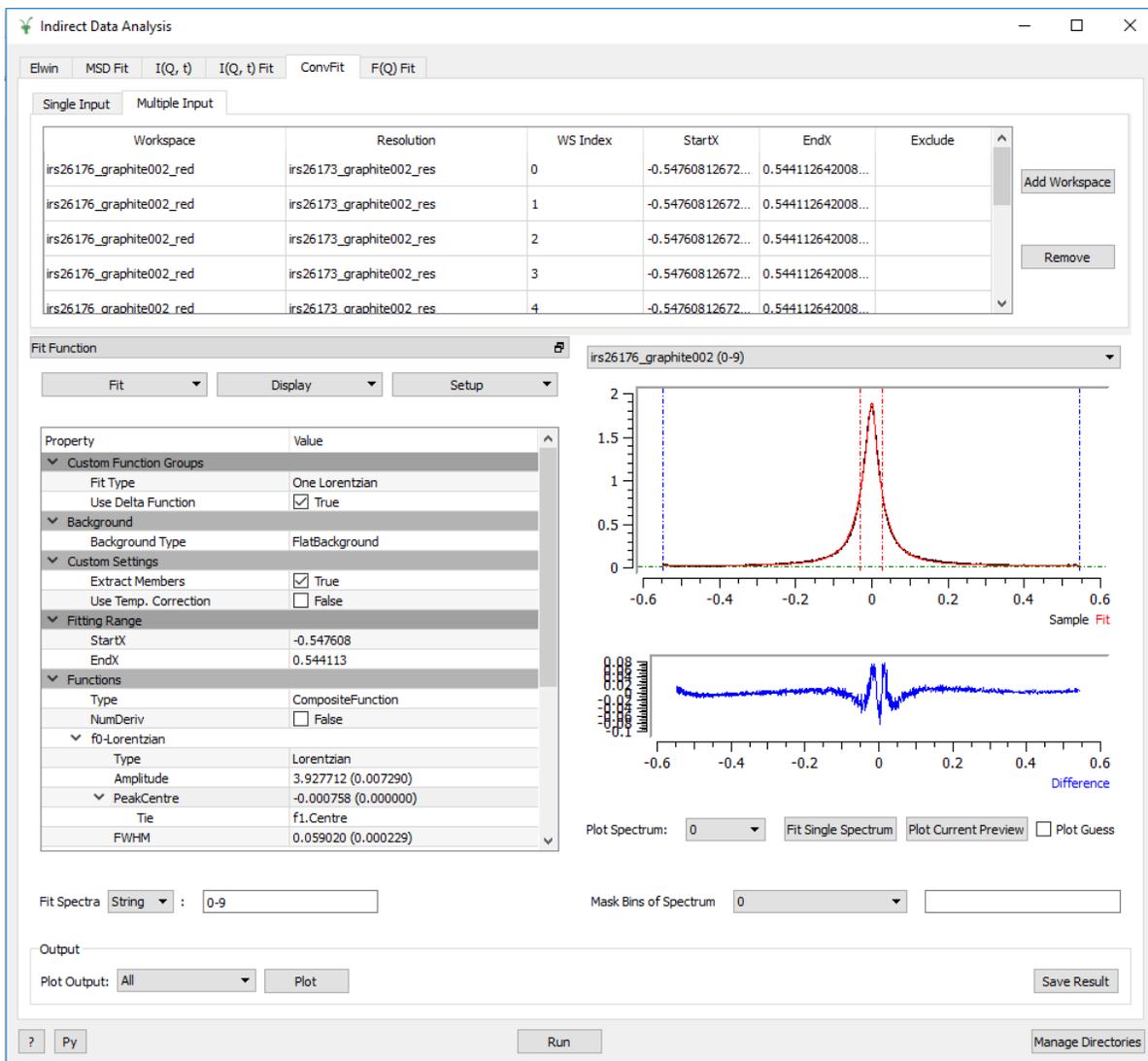
Figure 22: The 'ConvFit' interface in multiple-input mode
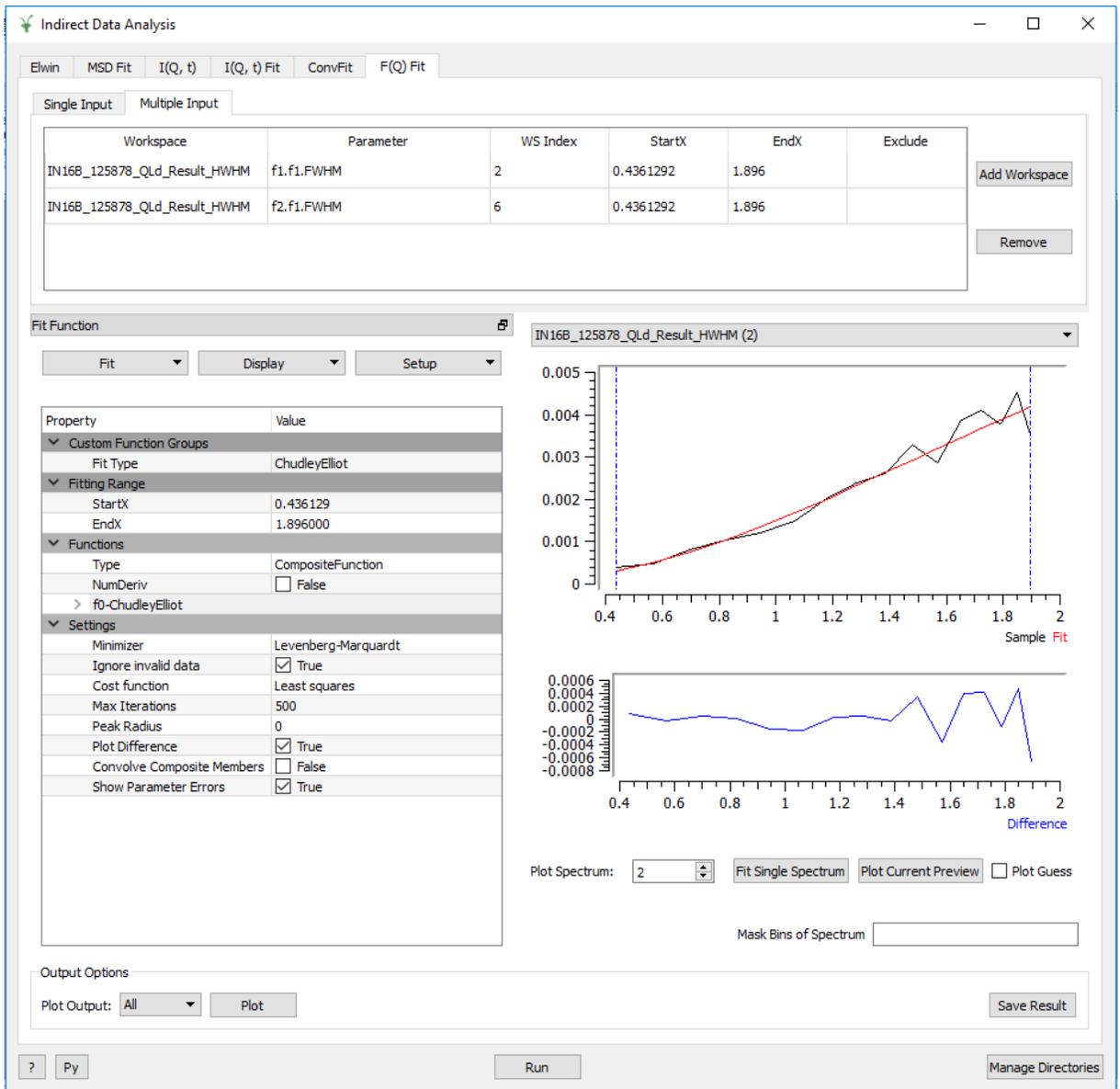
Figure 23: The '$F(Q)$' Fit interface in multiple-input mode

In multiple dataset mode, a table displaying the selected datasets replaces the input data selection. Datasets can be selected in the table by clicking on them. Each row in the '$I(Q,t)$ Fit' and 'MSD Fit' tables contains the workspace name, resolution name, workspace index, start and end x-values

for fitting and the excluded x-regions. Each row in the 'ConvFit' table contains the same information as in '$I(Q,t)$ Fit' and 'MSD Fit' interfaces, with the addition of the resolution name found adjacent to the workspace name. Each row in the '$F(Q)$ Fit' table contains the same information as in '$I(Q,t)$ Fit' and 'MSD Fit' interfaces, with the addition of the parameter name found adjacent to the workspace name.

A drop-down menu, located above the plots, can be used to select the active workspace (the dataset shown within the interface). The active spectrum within the active workspace can be selected using the 'Plot Spectrum' drop-down menu. The parameter values in the browser and the plots will be updated to reflect the active spectrum within the active workspace.

The 'Add Workspace' button, adjacent to the table, can be used to bring up a dialog box for selecting input data. The 'MSD Fit' and '$I(Q,t)$ Fit' dialog boxes (Figure 25) provide input fields for the input workspace and the spectra to add. The 'ConvFit' dialog box (Figure 24) provides input fields for the input workspace, resolution and the spectra to add. The '$F(Q)$ Fit' dialog box (26) provides input fields for the input workspace, parameter type and parameter name. The 'Remove' button, found below the 'Add Workspace' button, will remove all selected datasets from the table.
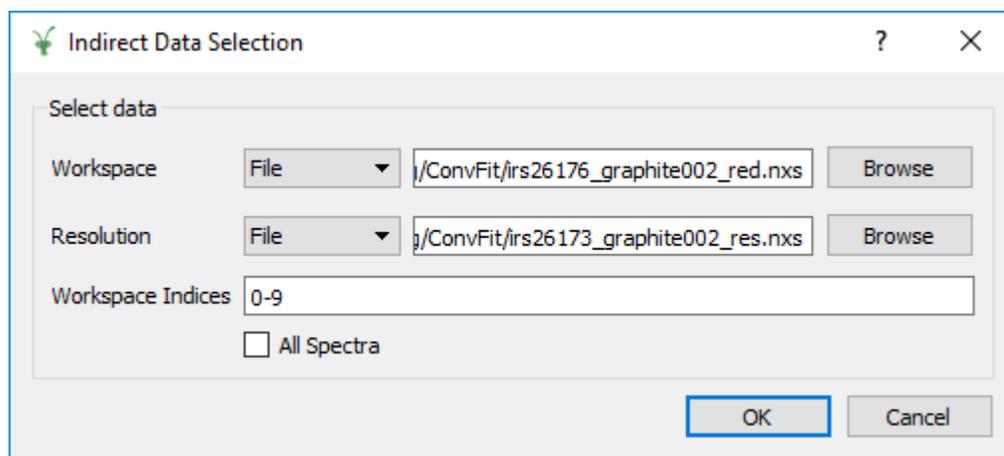
Figure 24: The pop-up menu presented for selecting data in 'ConvFit', when in multiple input mode

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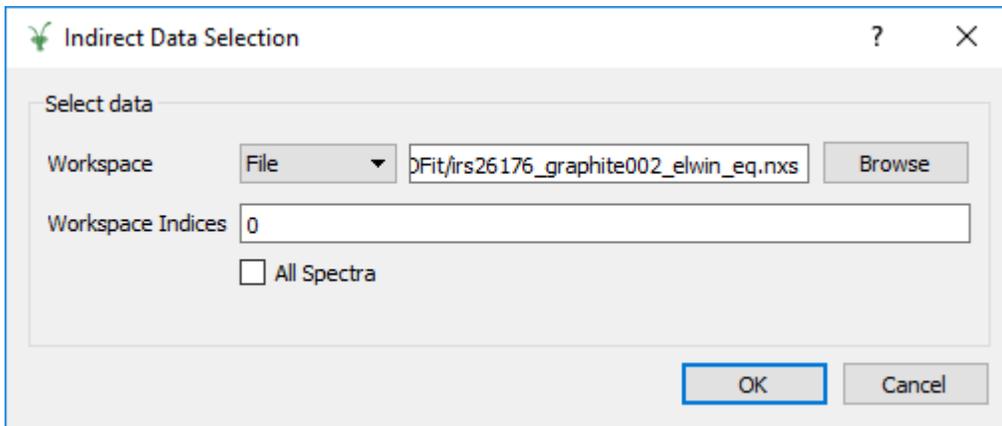
Figure 25: The pop-up menu presented for selecting data in '$I(Q,t)$ Fit' and 'MSDFit', when in multiple input mode
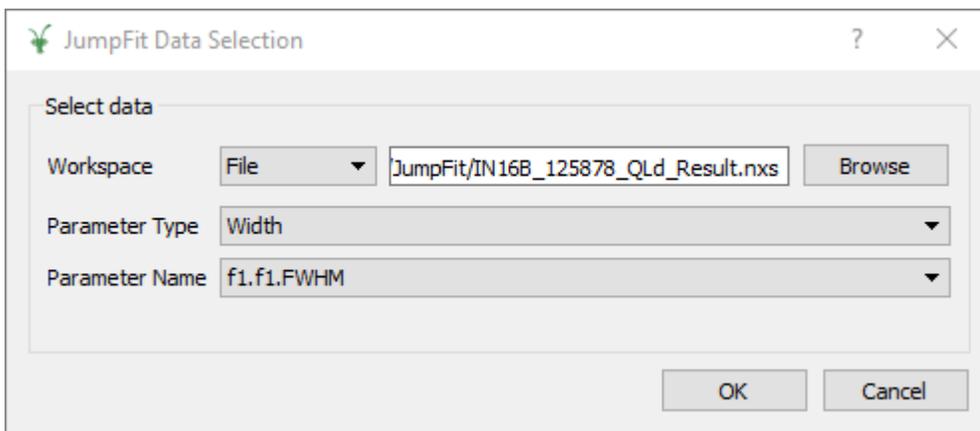
Figure 26: The pop-up menu presented for selecting data in '$F(Q)$ Fit', when in multiple input mode

6 OSIRIS Diffraction

In MANTID version 3.12, the 'Detect D-Range' and 'DRange' properties' of the 'OSIRISDiffractionReduction' algorithm have been removed. The x-range (domain) of the input workspace supplied to the 'OSIRISDiffractionReduction' algorithm is now automatically mapped to the corresponding

d-range.

Sample, container and vanadium runs supplied to the 'OSIRISDiffractionReduction' algorithm are now collected together by d-range, as opposed to being collected by the order they were supplied in. The smallest overlapping subset of d-ranges of the provided sample, container and vanadium runs is used in the reduction routine.

The 'OSIRISDiffractionReduction' algorithm can be accessed by opening the indirect diffraction reduction interface in MANTID, selecting 'OSIRIS' as the instrument and 'diffonly' as the reflection mode (see Figure 27). The 'ISISIndirectDiffractionReduction' algorithm is used when 'diffspec' is selected (see Figure 28).
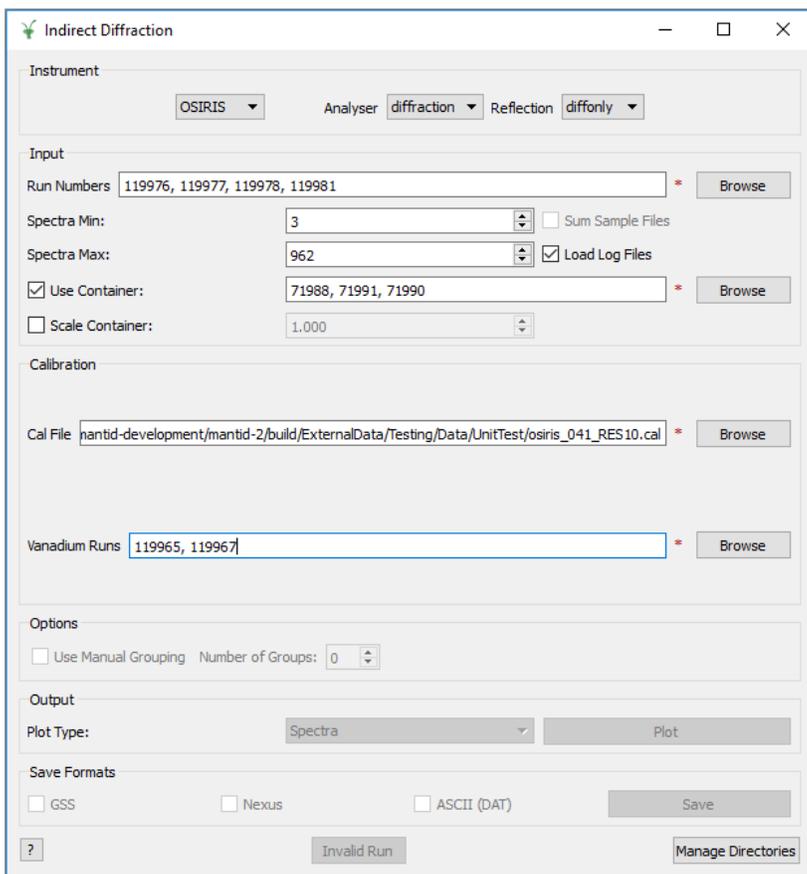
Figure 27: The indirect diffraction interface in 'diffonly' mode for the OSIRIS instrument
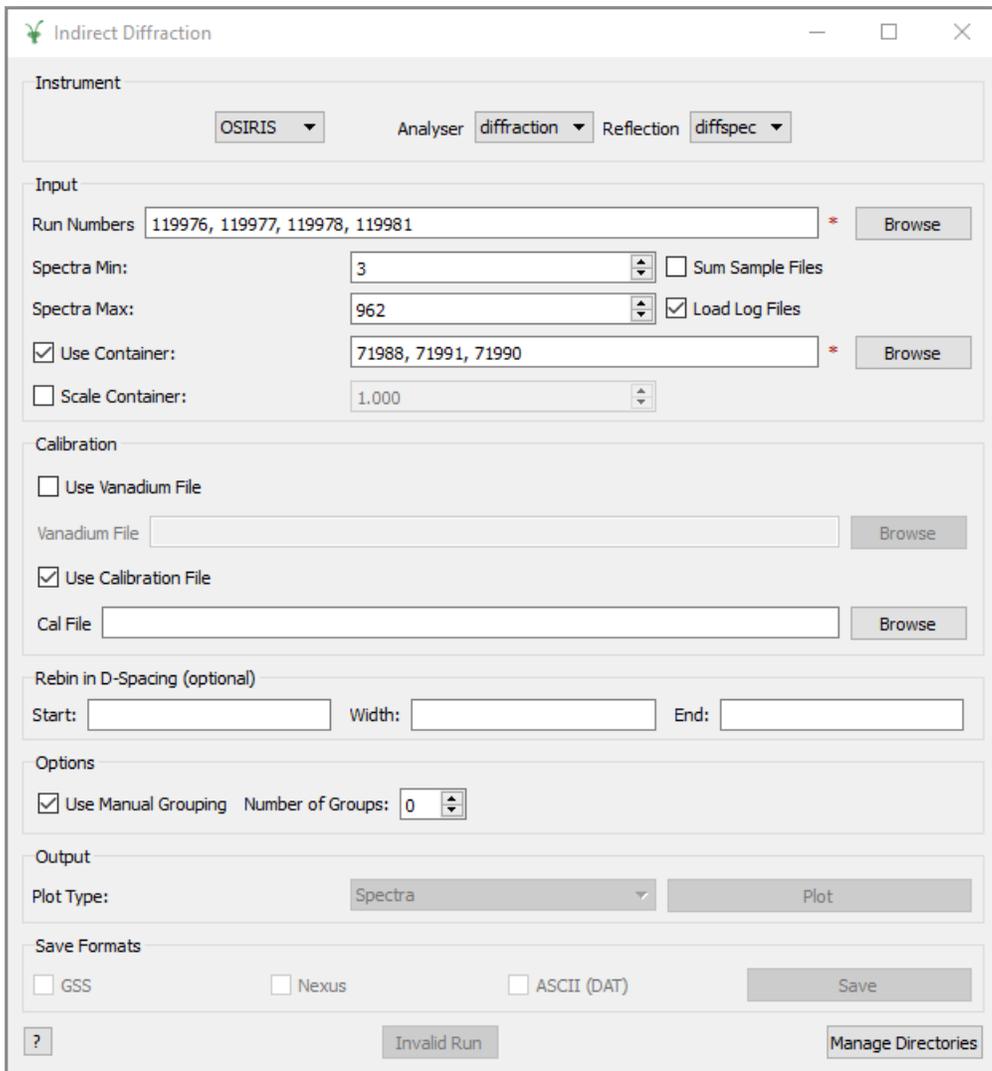
Figure 28: The indirect diffraction interface in 'diffspec' mode for the OSIRIS instrument

7 CAAD on Vesuvio

The cumulative angle-averaged data (CAAD) routine for the VESUVIO instrument [11] can be applied by setting the 'calculate_caad' flag to true in the VESUVIO driver script, as of MANTID version 3.12. This routine nor-

malises the results of each fitting iteration by their integral and then sums the normalised results, with the potential to increase the information content of the Neutron-Compton scattering data.

8   Prospective Developments

8.1   Simultaneous fitting in QENS interfaces

Simultaneous fitting is unavailable within the QENS fitting interfaces in MANTID version 3.13. The addition of simultaneous fitting to the QENS fitting interfaces is under development and will allow creating ties between the parameters of different spectra. Simultaneous fitting within the QENS fitting interfaces will replicate the behaviour of that found in the 'Multiple Dataset Fitting' interface in MANTID.

8.2   Relocating calculation of cumulative angle-averaged data

The cumulative angle-averaged data calculation for the VESUVIO data instrument, is currently integrated into the routine used by the the VESUVIO driver scripts. This calculation should be integrated into the 'VesuvioTOF-Fit' algorithm within MANTID, allowing for its use outside of the driver script.

References

[1] Mantid. Mantid: Manipulation and Analysis Toolkit for Instrument Data., Mantid Project. `http://www.mantidproject.org/Main_Page`, 2013.

[2] S. Howells D. Nixon and S. Mukhopadhyay. An Introduction to Inelastic Neutron Scattering and MANTID at ISIS, 2015.

[3] D. Nixon. Developments in MANTID relating to indirect inelastic spectroscopy between July 2014-July 2015. Technical Report RAL-TR-2015-007, STFC, 2015.

[4] E. Oram and L. McCann. Developments in MANTID relating to indirect inelastic spectroscopy between July 2015-July 2016. Technical Report RAL-TR-2016-019, STFC, 2016.

[5] L. McCann. Developments in MANTID relating to indirect inelastic spectroscopy between July 2016-July 2017. Technical Report RAL-TR-2017-012, STFC, 2017.

[6] H. H. Paalman and C. J. Pings. Numerical Evaluation of XRay Absorption Factors for Cylindrical Samples and Annular Sample Cells. *Journal of Applied Physics*, 33(8):2635–2639, 1962.

[7] SimpleShapeMonteCarloAbsorption v1. `http://docs.mantidproject.org/nightly/algorithms/SimpleShapeMonteCarloAbsorption-v1.html`, 2017. Accessed: 2017-12-15.

[8] B. Hewer and L. McCann. Developments in MANTID relating to indirect inelastic spectroscopy between July 2017-December 2017. Technical Report RAL-TR-2018-002, STFC, 2018.

[9] Judith Peters and Gerald R. Kneller. Motional heterogeneity in human acetylcholinesterase revealed by a non-Gaussian model for elastic incoherent neutron scattering. *The Journal of Chemical Physics*, 139(16):165102, 2013.

[10] Zheng Yi, Yinglong Miao, Jerome Baudry, Nitin Jain, and Jeremy C. Smith. Derivation of Mean-Square Displacements for Protein Dynamics

from Elastic Incoherent Neutron Scattering. *The Journal of Physical Chemistry B*, 116(16):5028–5036, 2012. PMID: 22471396.

[11] Maciej Krzystyniak, Selena E. Richards, Andrew G. Seel, and Felix Fernandez-Alonso. Mass-selective neutron spectroscopy of lithium hydride and deuteride: Experimental assessment of the harmonic and impulse approximations. *Phys. Rev. B*, 88:184304, Nov 2013.