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Overview of developments in MANTID relating to Indirect Inelastic Spectroscopy.
July 2017 - December 2017

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Overview of Developments in MANTID relating to Indirect Inelastic Spectroscopy July 2017 – December 2017

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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 [Mantid, 2013].

This report provides an outline of the developments to the Indirect Inelastic neutron spectroscopy routines, within MANTID between the months of July and December 2017. Notable changes have been made to QENS data-analysis and corrections, including new Monte-Carlo procedures for calculating absorption corrections.

Contents

1 Acknowledgements

2   Introduction

The MANTID project is a cross platform, open source framework which supports the manipulation of scientific data. 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.

3 QENS Data Analysis

3.1 Elastic window

The 'ElasticWindowMultiple' algorithm within MANTID is used to run the 'ElasticWindow' reduction algorithm, over a set of workspaces, and appends each result to an output MANTID workspace. This algorithm produces an output in Q and Q^2, in the same manner as the 'ElasticWindow' algorithm. 'ElasticWindowMultiple' produces extra output in the form of the sorted transposition of the output in Q. This extra output is then used to produce a fourth output, which was previously produced by normalising by the first temperature found within the sample logs. Normalisation now uses the lowest temperature found within the sample logs.

Normalisation in the 'ElasticWindowMultiple' algorithm, as of MANTID version 3.12, propagates errors within the input through to the output. This is achieved using the formula,

$$\sigma_{\text{out}}(x)^2 = \lambda^2 \left(\sigma_{\text{in}}(x)^2 + \left(\lambda Y(x) \sigma_{Y(c)} \right)^2 \right), \tag{1}$$

where
$Y(x)$ is the y-value at x in the input,
$\sigma_{\text{in}}(x)$ is the error-value at x in the input,
$\sigma_{\text{out}}(x)$ is the error-value at x in the output,
σ_y is the error-value on the output y,
c is a constant, user defined value in the input,
$\lambda = \frac{1}{Y(c)}$

3.2 Convolution fit

Extracting the members used within a fit has been implemented within the convolution fitting routines. Members are defined to be the functions used in the fit; this includes a delta function, if one was used. This new feature has an impact on both the convolution fit algorithm and the user interface.

The convolution fit algorithm, known as 'ConvolutionFitSequential' within MANTID, has been provided with a new property; 'ExtractMembers'. The 'ExtractMembers' property is defined as a boolean value which when evaluated as true will result in the algorithm extracting the fit members. The values for each member of the fit, across all spectra selected to be fit, are

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used to create a MANTID workspace. Each of these member workspaces then have their y-axis set to the momentum values found within the input quasi-elastic neutron scattering data.

As of MANTID version 3.11, a check-box has been added to the property table within the indirect, convolution fit interface. This check-box has been provided with the label 'ExtractMembers', matching the newly defined property in the 'ConvolutionFitSequential' algorithm. The value of this check-box (true if checked, false otherwise) is passed to the 'ExtractMembers' property of the fit algorithm.

It is now possible to plot a guess fit for the diffusion functions within the convolution fit interface. A guess fit is created by taking the values for the model parameters, defined by the user in the interface, and using the selected model to calculate the y-values (range) from a selected set of x-values (domain).

3.3 Peters and Yi models for Mean-squared displacement fit

Two new models, for mean-squared displacement fitting, have been identified and included within MANTID version 3.11: Peters model [Peters and Kneller, 2013] and Yi model [Yi et al., 2012]. To provide a method for selecting the model to use, the mean-squared displacement fit algorithm (named 'MSDFit' in MANTID) has been given an additional property; 'Model'. The 'Model' property can currently take one of three values: 'Gauss', 'Peters', 'Yi'. The values of the 'Model' property correspond to a Gaussian decay function, the Peters model and the Yi model, respectively. As a result of the addition of two new models, the indirect mean squared displacement fit interface now includes a drop-down menu for selecting which model to fit.

The plot guess feature, as seen in all other indirect fit interfaces within MANTID, has now been included within the mean squared displacement fit interface.

3.4 General improvements

The indirect fit analysis interfaces, as of MANTID version 3.12, now have two separate preview plots, laid out vertically. The top preview plot displays the input data and the result of a fit. The bottom preview plot displays

the difference between the input data and the fit. Figure 1 depicts the new plotting component of the indirect fitting interfaces.
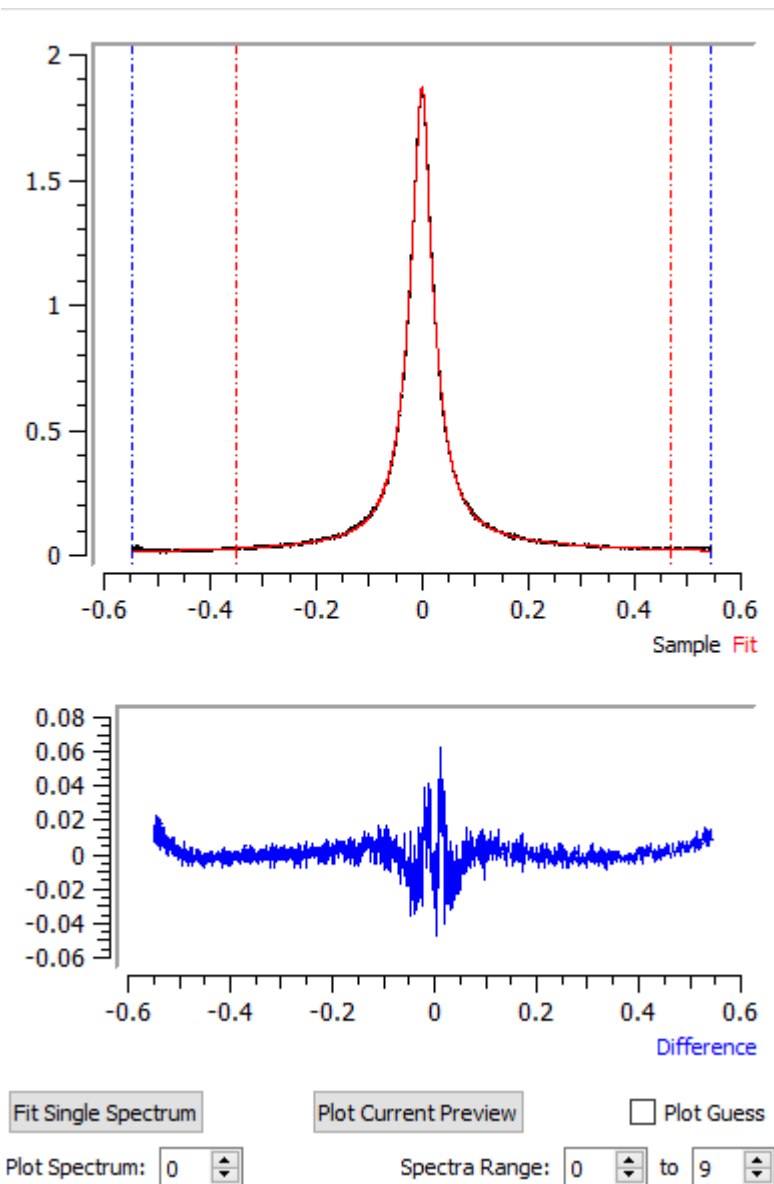

Figure 1: Image of the new design of the plotting functionality within the indirect fitting interfaces

4 Diffraction

The ability to save the reduced data, produced by the indirect diffraction algorithms, by way of the user interface, was previously not functioning for OSIRIS in diffraction-only mode. The ability to save in GSS format now functions as expected, across all diffraction modes, as of MANTID version 3.11.

The indirect diffraction reduction interface, within MANTID, previously displayed a check-box with the label 'Use Individual Grouping'. In the case where this check-box was checked, the results of the reduction routines would be grouped into a single spectrum.

The 'Use Individual Grouping' check-box has been changed to 'Use Manual Grouping' in MANTID version 3.11. In the case where this check-box is checked, a number field will become available, where the number of groups, to create in the grouping process, may be selected by a user.

The indirect diffraction reduction interface previously included a check-box labelled 'Sum Files'. If the 'Sum Files' check-box was checked, the sample and vanadium runs specified within the interface, would both be summed. The result of these summations, would then be passed to the diffraction reduction algorithms.

As of MANTID version 3.11, the 'Sum Files' check-box has been renamed to 'Sum Sample Files' and the behaviour when this check-box is checked has been altered. The vanadium runs are now left unchanged, rather than being summed. The sample runs are evaluated in the scheme laid out by Table 1.

Input Syntax	Description of Evaluation
A	Passes sample run A to the appropriate reduction algorithm
A-B	Sums the range of sample runs from run A to run B and passes the result to the appropriate reduction algorithm
A+B	Sums sample run A and sample run B and passes the result to the appropriate reduction algorithm
A:B	Passes each sample run in the range A to B individually to the appropriate reduction algorithm
E_1,E_2	Evaluates expression E_1 and E_2 separately (recursive definition)

Table 1: Detailing how the sample runs input in the indirect diffraction reduction interface is evaluated, when the 'Sum Files' check-box is checked

The 'Detect D-Range' and 'DRange' properties of the 'OSIRISDiffractionReduction' algorithm, have been removed in MANTID version 3.12. The d-ranges for sample, container and vanadium data, can be automatically extracted using the x-range (domain) found within the data. This is true, as there is a one to one correspondence between the x-range and the d-range of a run, given the properties of the diffraction instrument remain constant.

Sample, container and vanadium runs supplied to the 'OSIRISDiffractionReduction' algorithm, are now associated by their d-ranges (automatically found), as opposed to being associated by their position in a character string. The smallest overlapping subset of d-ranges of the provided sample, container and vanadium runs is used in the reduction routine.

The 'Use Manual D-Range' check-box, previously found in the indirect diffraction reduction interface, when 'OSIRIS' was selected as the instrument, has been removed.

5 QENS Corrections

5.1 Paalman-Pings method for absorption corrections

Absorption corrections, for indirect inelastic data within MANTID, are calculated using the numerical evaluation method outlined by Paalman and

Pings [Paalman and Pings, 1962]. This method outlines an approach to calculating absorption corrections, using a set of absorption factors, these are detailed in Table 2.

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 2: Description of the Paalman-Pings absorption factors

The standard application of the Paalman-Pings absorption factors, in order to correct for absorption, is as follows:

$$I_s = \frac{1}{A_{s,sc}} \left(I_{sc}^E - K_c I_c^E \frac{A_{c,sc}}{A_{cc}} \right) \tag{2}$$

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

In the circumstance in which a container is not used, the application is as follows:

$$I_s = \frac{I_s^E}{A_{s,s}}, \tag{3}$$

where I_s^E is the sample data before corrections are applied.

5.2 Monte Carlo method for calculating Paalman-Pings absorption factors

Within MANTID, a Monte Carlo algorithm (named 'MonteCarloAbsorption') can be used for calculating an absorption factor from supplied input data, in the form of a MANTID workspace. The input workspace will contain the information describing the neutron beam and the material the neutron will pass through (geometry and composition).

The 'MonteCarloAbsorption' algorithm first generates a random starting position within the beam. A random scattering point is then generated, within the material. The path taken by the neutron is calculated and the absorption of the neutron, taking into account the attenuation factor, is calculated along that path. This simulation is run several times and the results are accumulated and averaged.

The current version of the 'MonteCarloAbsorption' algorithm is unable to handle multiple regions, in which the scattering event is restricted to only one of them. Sample data, with the container information (geometry and composition) included, will produce a single correction factor when passed to the 'MonteCarloAbsorption' algorithm. During the creation of the output correction factor, for each simulation, a scattering event could have occured in either the sample or container. It is therefore currently not possible to calculate the $A_{s,sc}$ and $A_{c,sc}$ factors, using the 'MonteCarloAbsorption' algorithm.

5.3   Simple shape Monte Carlo absorption corrections

Providing users of MANTID with a method of defining the shape of the sample and container, prior to calling the 'MonteCarloAbsorption' algorithm, has been included in version 3.11. A new algorithm, 'SimpleShapeMonteCarloAbsorption', incorporates properties for defining the shape of the material within the input data.

The 'SimpleShapeMonteCarloAbsorption' algorithm, first defines the geometry on the input workspace, using the defined shape properties. The algorithm subsequently performs a call to the 'MonteCarloAbsorption' algorithm and sets the 'OutputWorkspace' property to the result. Further details of this new algorithm can be found on its MANTID documentation page [SimpleShapeMonteCarloAbsorption, 2017].

5.4   Indirect Monte Carlo absorption corrections

An indirect specific Monte Carlo absorption correction algorithm has been created, for MANTID version 3.11, with the name 'CalculateMonteCarloAbsorption'. This algorithm provides a single interface for calculating the $A_{s,s}$ and $A_{c,c}$ correction factors.

The 'CalculateMonteCarloAbsorption' algorithm provides properties for setting the sample data and shape as well as the empty container data and

shape. Both the sample and container workspace are converted into units of wavelength. The sample workspace and the sample shape information are passed into the 'SimpleShapeMonteCarloAbsorption' algorithm, in order to calculate the $A_{s,s}$ workspace. The container workspace and the container shape information are passed into the 'SimpleShapeMonteCarloAbsorption' algorithm, in order to calculate the $A_{c,c}$ workspace. Further details of this new algorithm can be found on its MANTID documentation page [CalculateMonteCarloAbsorption, 2016].

A new indirect corrections user interface, 'Calculate Monte Carlo', has also been added in MANTID version 3.11 (depicted in Figure 2). This interface provides a graphical way of accessing the 'CalculateMonteCarloAbsorption' algorithm.

5.5   Applying two-factor Paalman-Pings approximation

In order to apply the two Paalman-Pings factors $(A_{c,c}, A_{s,s})$ produced by the 'CalculateMonteCarloAbsorption' algorithm, a revised approximation was used. This approximation is formulated as follows,

$$I_s = \frac{I_{sc}^E}{A_{s,s}} - K_c \frac{I_c^E}{A_{c,c}}, \tag{4}$$

where I_{sc}^E is the input sample data,
I_c^E is the input container data,
K_c is the container scale factor,
$A_{s,s}$ and $A_{c,c}$ are defined in Table 2.

The existing algorithm for applying the Paalman-Pings absorption factors, 'ApplyPaalmanPings', has been modified to use the best approximation, given a set of correction factors. In the circumstance where either the $A_{s,sc}$ or $A_{c,sc}$ correction factors are not provided, the two-factor approximation described above will be used. This is true as of MANTID version 3.12.

5.6   Restructured layout

The layout of the corrections interface has been restructured, in order to accommodate the introduction of the new simple shape monte-carlo method for the calculation of absorption corrections. The new layout is depicted in Figure 2.

Figure 2: Image of the new layout of the indirect corrections interface; the Calculate Monte Carlo Absorption interface is also presented

6 VESUVIO

The incident angles for neutrons scattering off hydrogen atoms lie outside of the 133-165 degree angular range of the VESUVIO back-scattering detectors. Consequently, the impact of the hydrogen peak is not recorded within the raw time-of-flight (ToF) data.

To account for the hydrogen peak, the VESUVIO data analysis routines, as of MANTID version 3.11, compute an approximation using the composition of the material, as defined by user-supplied constraints within a driver script. These constraints are applied as follows;

$$I_H = \sum_{i=1}^{N} \frac{\sigma_H}{\sigma_{M_i}} \mu_{M_i} \sigma_{M_i},$$

(5)

where
σ_x is the neutron scattering cross-section of mass x,
μ_x is the constraint value supplied, by the user, for mass x,
M_i is the mass used in the ith constraint,
N is the number of supplied constraints,
I_H is the approximated intensity of the hydrogen peak.

Time-of-flight data loaded by the VESUVIO loader ('LoadVesuvio' in MANTID, can now be loaded without the sample logs. In order to achieve this, the 'LoadVesuvio' algorithm has been given an additional boolean property, in MANTID version 3.12; 'LoadLogFiles'. When this property is set to a false value, the sample logs will not be loaded into the time-of-flight data.

Currently, the sample and container runs to be loaded must be passed to the VESUVIO fit routines, within the VESUVIO driver script. As of MANTID version 3.12, it is possible to instead supply pre-loaded workspaces, by setting the 'sample_runs' and 'container_runs' flags to the appropriate workspaces.

7   Prospective Developments

7.1   Improving the Monte Carlo method for calculating absorption factors

As described in section 5.2, the Monte Carlo method, as used for calculating the Paalman-Pings correction factors, is only able to produce the $A_{s,s}$ and $A_{c,c}$ factors. The 'MonteCarloAbsorption' algorithm, will be adapted in the future, to have the capacity to consider multiple regions and restrict where the scattering occurs. This adaptation will allow for producing the three correction factors required for the three-factor Paalman-Pings application.

7.2   Extending functionality in QENS-fitting

A range of fitting functionality remains absent from the QENS-fitting interfaces, including custom parameter ties, constraints and adding custom as well as user-defined functions. Selecting discontinuous spectra ranges and masking defined ranges in the fit is also currently not available. These features are currently in development within the MANTID framework. In addition, the QENS-fitting interfaces are currently limited to single datasets, with future developments planning to bring the option of fitting across multiple datasets.

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