QENS Data Analysis in Mantid
Past, Present and Future

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Motivation

- A single software for reduction, visualizations and analysis of QENS data across all international facilities.

- Taking out the QENS spectroscopy from the concept of expert only technique to present to all scientists, particularly for industrial users, with the aim of expanding the users’ group.

- An open source sustainable software, easy to use, easy to upgrade, easy to contribute.
### QENS Data Analysis in Mantid: History

<table>
<thead>
<tr>
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**Note:** The diagram shows the history of QENS data analysis in Mantid, with key developments and their associated years and sites.
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**OpenGenie**

**IDL**

**C++**
QENS Data Analysis in Mantid: History


2011: QENS fitting in Mantid (ISIS)
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2017: SINE2020 QENS fitting in Mantid
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OpenGenie IDL IDL C++ Python

Python C++ MVP pattern
Matplotlib Python plotting as GUI
### QENS Data Analysis in Mantid: History

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- Nine RAL Technical reports
- On-line Mantid documentation pages
- Mantid QENS Manual
- GUI
- Tailored for IRIS and OSIRIS- QENS instruments at ISIS

**Technologies**
- OpenGenie
- IDL
- IDL
- C++

**Software**
- Python
- C++
- Matplotlib
- MVP pattern

**Tools**
- GUI
SINE2020 timeline regarding software for QENS data analysis

Following the SINE2020 WP10 workshop II at ILL (2017), a dedicated workshop was held at ISIS to discuss the requirements and design principles of QENS fitting GUI.

QENS Fitting Workshop, 11-12th Sept, 2017

Following a video meeting, international requirements are gathered in February, 2018.

SINE2020 supported the idea of implementing the QENS fitting GUI within Mantid.

The development update was presented in the workshop III, at Soragna in 2018.
Requirements for QENS Fitting GUI

- Simultaneous fitting of Q-dependent spectra and multiple data sets
- Simple, but complete methods to apply constraints and link fit parameters
- Accept input from multiple instruments or formats
- Provide methods to estimate fit reliability
- Comparison of different fits
- Extensive library of models and possibility to add easily new models
- Possibility to choose between different fitting methods (LM, MC, Bayes,..)
- Intuitive GUI, but possibility to fit from command line
- Able to save and load complete session
- Access to low level for experts
- Publication quality plots
- Extensive documentation, including examples and tutorials
  - Able to fit in background using multiple cores or cluster
  - Fourier Transform of input data (fitting in $\omega$ and in time), handle multiple scattering, possibility of reducing the weight of the elastic peak in the fit, fit both QENS and fixed window scan data, ...
QENS Fitting GUI – The Plan

Draft mockup for QENS fitting GUI for multiple data set fitting: Model 1

Select fitting domain energy ($S(Q,w)$) or time ($I(Q,t)$)

Select fitting function/models suitable for energy ($S(Q,w)$) or time ($I(Q,t)$) and background
(This should be connected with model library)

Masking option for particular $Q$ to remove Bragg peaks

Control over fitting parameters, $X$ is either energy or time

Start fitting

Help button to link with documentation

Load sample (reduced) data

Load resolution/vanadium data
(A default vanadium data for the instrument can always be in loaded mode, but users will get options to load their own resolution file (sample data from base temperature))

Area to display, loaded data, fitted curves as well as guess plots

Area to plot residuals

Plot options (to be changed according to energy domain or time domain fittings)

Plot of $\chi^2$
QENS Fitting GUI – The Plan

Draft mockup for QENS fitting GUI for multiple data set fitting: Model 2

- Load sample (reduced) data
  - Load resolution/vanadium data (A default vanadium data for the instrument can always be in loaded mode, but users will get options to load their own resolution file (sample data from base temperature)

- Select fitting domain energy \( S(Q,w) \) or time \( I(Q,t) \)

- Masking option for particular Q to remove Bragg peaks

- Control over fitting parameters, X is either energy or time

- Start fitting

- Saving and Export options

- Help button to link with documentation

- Area to display, loaded data, fitted curves as well as guess plots

- Workspace for files

- All tile plots should open in separate windows

- Area to plot residuals

- Area to plot FWHM – \( Q^2 \)

- Area to plot \( \chi^2 – Q \)
QENS Fitting GUI – The Plan

**QENS MD FITTING**

### Load data

<table>
<thead>
<tr>
<th>Scattering data</th>
<th>Resolution data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enter filename(s) or workspace name(s)</td>
<td>Enter filename(s) or workspace name(s)</td>
</tr>
<tr>
<td>Browser</td>
<td>Browser</td>
</tr>
</tbody>
</table>

- **Load**
- **Reduce**
- **Fit**

### Summary of loaded data

<table>
<thead>
<tr>
<th>Data</th>
<th>Resolution File</th>
<th>Select for reduction</th>
</tr>
</thead>
<tbody>
<tr>
<td>dataset1</td>
<td>IRF1</td>
<td>□</td>
</tr>
<tr>
<td>dataset2</td>
<td>IRF2</td>
<td>✓</td>
</tr>
<tr>
<td>workspace_a</td>
<td>IRF1</td>
<td>□</td>
</tr>
<tr>
<td>workspace_b</td>
<td>IRF1, IRF2</td>
<td>✓</td>
</tr>
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- **Scrolling through plots of raw data**
- **Select data to plot**
- **Save**
- **Close**
- **Help**

- Right-click to remove loaded data
- Association between scattering data and resolution data
- Selection of sets to be treated (reduction / fitting)
QENS Fitting GUI – The Plan
QENS Fitting GUI – The Design

- The interface was refactored for easy access to GUI and low level
- Model View Presenter (MVP) Pattern for easy upgrade
- All fittings are free from instrument parameters for portability to different facilities
- Extensive development in MD fitting simultaneously, Q dependent fitting,
- Mostly in python
Present
QENS Data Analysis in Mantid
Mantid version 3.4

https://www.mantidproject.org/Indirect:Indirect_Data_Analysis
QENS Data Analysis GUI in Mantid

Elastic window scan

\[
\int_{-E_1}^{E_1} S'(Q, E) dE
\]

http://docs.mantidproject.org/nightly/algorithms
/ElasticWindowMultiple-v1.html
QENS Data Analysis GUI in Mantid
QENS Data Analysis GUI in Mantid
$I(q,t) = \text{FT}[S'(Q, E)]$

Error calculations are done by using Monte Carlo method.
I(q,t) Fit

Available functions
- Exponential
- Two exponentials
- Stretched exponential
- One stretched + exponential
QENS Data Analysis GUI in Mantid

Convolution Fit

Available functions
- Lorentzian
- Two Lorentzians
- Inelastic diff sphere
- Inelastic diff rotation circle
- Elastic diff sphere
- Elastic diff rotation circle
- Stretched exponential FT
Available functions

F(Q) Fit:  
FWHM fit  
EISF fit

EISF Fit:
- Diffusion in sphere
- Diffusion in cylinder
- Diffusion in long chain molecules
Documentations and Tutorials

Mantid Documentation
https://docs.mantidproject.org/nightly/interfaces/Indirect%20Data%20Analysis.html

Mantid QENS User’s Guide
https://www.isis.stfc.ac.uk/Pages/Mantid-QENS-Manual-online-Content.aspx

Mantid QENS Tutorial
https://lmsdevweb.stfc.ac.uk/moodle/course/view.php?id=149

Publications:
Future
Mantid Developments

The Mantid developments from ISIS will be driven by instrument scientists

Mantid workbench compatibility

More fitting functions

Fitting with Q
Mantid 4

Mantid workbench is designed to be more user friendly and more stable than MantidPlot.

Plotting in workbench is now matplotlib.

None of the indirect inelastic interfaces are currently available.
We will be porting the indirect interfaces to workbench.

This is a non-trivial task due to the embedded plotting.

Aim to have all of the interfaces ported for Mantid 4.2.
More fitting functions

The QENS library\(^1\) has a set of fitting functions.

Can import them into Mantid for analysis

\(^1\) https://github.com/QENSlibrary/QENSmodels
More fitting functions

Out of the box can be used like any other Python function

Not compatible out of the box with Mantid’s fitting
More Mantid fitting functions

Can write simple wrapper scripts to expose the QENS library to Mantid

```python
from mantid.simpleapi import *
import QENSmodels

# wrap to create mantid fitting function
class sqwChudleyElliotDiffusion(IFunction1D): # or IPeakFunction
    def init(self):
        self.declareParameter("scale", 1.0)
        self.declareParameter("center", 0.0)
        self.declareParameter("D", 0.23)
        self.declareParameter("L", 1.0)
        self.declareParameter("Q", 0.1)

    def category(self):
        return 'QuasiElastic'

    def function1D(self, xvals):
        scale = self.getParameterValue("scale")
        center = self.getParameterValue("center")
        D = self.getParameterValue("D")
        L = self.getParameterValue("L")
        q = self.getParameterValue("Q")
        return QENSmodels.sqwChudleyElliotDiffusion(xvals, q, scale=scale, center=center, D=D, L=L)

# add it to Mantid fitting functions
FunctionFactory.subscribe(sqwChudleyElliotDiffusion)
```
More Mantid fitting functions

Can use the fitting functions like any other fitting function in Mantid
The Q value should be fixed for a given spectrum.

Want large statistics to improve quality of the fit.
Fitting with Q

Solution is fitting with fixed Q values

Gives good results for this example
How to get these

In the Mantid script repository

Users can add their own scripts

Can set Mantid to automatically run the scripts on start up
Summary

- Most of the functionality of QENS data analysis is available in Mantid in the form of GUI and algorithm.

- Further development on Bayesian analysis is ongoing for analysing complicated data consists of several overlapping peaks and backgrounds.

- More robust analysis exploiting simultaneous fitting and integration with QENS fitting model library is ongoing.
Acknowledgements

- Spencer Howell
- Robert Applin
- Brandon Hewer
- Dereck Tendachi Kachere
- Samuel Jackson
- Dan Nixon
- Elliot Oram
- Louise McCann
- Bartomeu Llopis Vidal
- Diego Monserat
- Roman Tolchenov
- Luis Carlos Pardo
- Felix Fernandez-Alonso

- Universitat Polit`ecnica de Catalunya and the UK Science & Technology Facilities Council for their continued support of this collaborative work

- Mantid team at ISIS for helping the implementation

- Friendly Users group of Molecular Spectroscopy for testing all implementation patiently

- SINE2020 for funding

Thank you for your attention!