Requirements of MD-QENS Fitting

October, 2017 – discussion with Heloisa Bordallo at ESS DMSC

Input January, 2018

- **Reorganization of short- and long-term goals**
- **Prioritisation of short-term goals**

Short Term Goals (1 year)

1) Control over spectrum number on the resolution function during convolution.
2) Control over fitting parameters, such as height and FWHM can be tied, fixed and varied within a range etc.
3) Sensible auto scaling for visualisation of fitted data with option to change scale.
4) Control over spectrum fitting, such as removing some Q from sequential fitting.
5) Option of saving data in ASCII format for plotting elsewhere.
6) Implementation of absorption corrections using various methods.
7) Multiple scattering corrections beyond Mayer's method and Paalman-Pings.
8) Fitting and analysis of multiple tunnelling peaks.
9) Global fits for rotational models etc.
10) Bayesian analysis of S(Q,E) using FABADA multi-dataset fit.
11) Detailed Tutorials
12) User defined model for fit and maintaining a model library

From the above list, the development procedure could be split into 2 parts depending on the largest users' community. From item5, there are 2 cases to distinguish (see schematic plot below):
- The reduced data do not require any additional corrections. In this case, basic fitting models can be used. The development can focus on the interface, fitting methods…
- Additional corrections are required. They have to be available from the interface
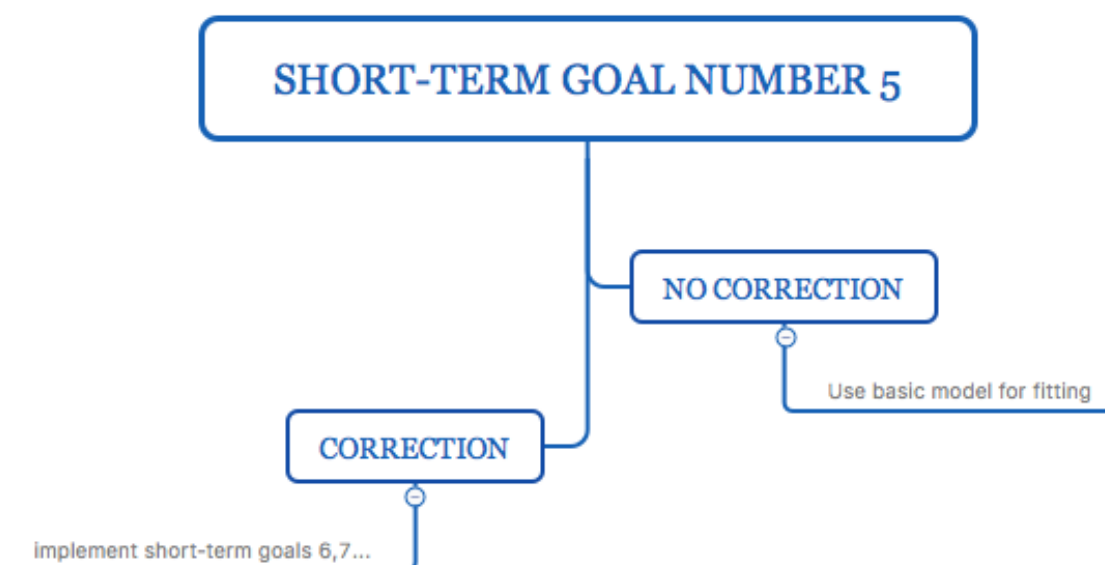
Medium Term Goals (2years)

- Flexible option to use in scripting as well as GUI mode.
- Publication quality plotting, preferably tiled, shifted/multiple X and Y axis, improved legends along with Mantid.
- More integration with simulations in data analysis and fitting.
- Multi-data set fitting interface irrespective of facility and computing platform
- Option for high throughput QENS analysis

QENS MD FITTING

Load | Reduce | Fit

Load data

Scattering data | Enter filename(s) or workspace name(s) | Browse   ⊘

Resolution data | Enter filename(s) or workspace name(s) | Browse   ⊘

☐ Use one resolution file or workspace for all data   **Load**   Help

Summary of loaded data ⊘

Data	Resolution File	Select for reduction
dataset1	IRF1 ▼	☐
dataset2	IRF2 ▼	☑
workspace_a	IRF1 ▼	☐
workspace_b	IRF1 ▼	☑
	IRF2	

⏪ ▶ ⏩   Select data to plot

Scrolling through plots of raw data

Plots of raw data with labels and units
Title of plotted workspace and spectrum

Save   Close   Help

Log / Progress bar

- Right-click to remove loaded data
- Association between scattering data and resolution data.
  Selection of sets to be treated (reduction / fitting)

QENS MD FITTING

Click to select
Right click to display
properties

Load Reduce Fit

Selected data

Reduction algorithms

Data	Resolution File	Rebin	Mask	Restore	Use script
dataset2	IRF2	☑	☐	☐	☐
workspace_b	IRF2	☐	☐	☐	☐

Give option to use a
Python script or to add
other algorithms to reduce
data

Reduction algorithm

Params Display default values

☐ Full Bins Only   ☐ Ignore Bin Errors   ☐ Preserve Events   [Apply] [Use default values] [Help]

Display characteristics of
selected algorithm or of
reduction script in Table
(for example here for
Rebin)

[Save reduction script]   [Display summary of reduction settings]   [**Reduce**]

Reduced data and history ⑦

Reduced dataset_1
  ▼ History
  ⊞ Rebin
Reduced workspace_b
  ▼ History

⏪ ▷ ⏩

Select data to plot

Scrolling through plots of reduced
data

Plots of reduced data with labels and units

[Save] [Close] [Help]

Log / Progress bar

Display list of **reduced** data with history of applied
algorithms

QENS MD FITTING

Load \ Reduce \ Fit

Fitting settings

Selected data

Data	Resolution File	Fit	Select spectra
dataset2	IRF2	☑	range
workspace_b	IRF2	☑	or single value

What to fit S(Q,w) ▼
I(Q)

Minimizer FABADA ▼ ⑦
☐ Edit minimizer parameters

Fitting model Gaussian ▼
Lorentzian
...
User defined

Background Linear ▼ ⑦
Polynomial

Fitting parameters

Model	Property	Value	Min	Max	Units	Fix	Tie	Constraints
Lorentzian	Amplitude	1.5	0	10	counts	☑	☐	☐
	FWHM	38	1	100	TOF	☐	☐	☐
	Center	0	-5	5	TOF	☐	☐	☐
Background	A0	0	-10	10	counts	☐	☐	☐

Display summary of fitting settings

Plot initial guess   **Fit**

Fitting results

Quality factor	Data/r (workspace)	Spectrum	Value
chi2	dataset2	3 ⬍	1.5
chi2	workspace_b	3 ⬍	38

⏪ ▶ ⏩   Select data to plot

Plots of reduced data & fitting models with labels and units (before or after fitting)

Display table of parameters for   Workspace / Spectrum ⬍

Save   Close   Help

Log / Progress bar

The table below will pop up once the workspace selected

Results - Fitting parameters for dataset2 spectrum 1

Model	Property	Value	Error	Units	Comments
Lorentzian	Amplitude	1.5	-	counts	fixed
	FWHM	20	1	TOF	
	Center	-2	0.2	TOF	
Background	A0	1	0.1	counts	

Plot fitting results   Close   Help