Requirements of Multi-Dimensional-QENS Fitting GUI
(February, 2018)

Overall goal:
To create and provide the user community with a user-friendly, comprehensive and general QENS fitting GUI in both reciprocal and real domains for neutron facilities.

Basic but Key Requirements:
- Control over all fitting parameters, such as amplitudes and FWHMs, so that they can be tied, fixed and varied within some specific value range etc.
- Control over which spectra to fit (eg. single, all, some specific ones required when some Bragg peaks want to be masked).
- Control over spectrum number on the resolution function during convolution
- Provision and maintenance of a model library for fitting common QENS observables and parameters (such as MSD, EISF, S(Q,E), I(Q,t), FWHM...). This should include outputting 'useful' variables for the user such as diffusion coefficients (in standard not neutron variables)
- Calculation of susceptibility and fits with common models (will help with joining data from different instruments)
- Provision to insert user defined models
- Calculation of EISF for basic one or, two Lorentzians for fitting.
- Simultaneous display of fit parameters (eg. amplitude, and FWHM in energy domain fitting,β and τ for time domain fitting) plus residuals ($\chi 2$) during fitting.
- Plot of HWHM with $Q2$ and EISF with Q
- Multiple dataset fitting for rotational models etc.
- Bayesian analysis of S(Q,E) data
- Fitting and analysis of tunnelling peak(s), alongside QENS broadening.
- Sensible auto scaling for visualisation of fitted data with option to change scale.
- Correct calculation of errors for all fitting algorithms
- Option of saving data in ASCII format for plotting elsewhere.
- Option for high throughput QENS analysis (ie. simultaneous/parallel analysis of similar samples which enables quick comparison of certain observables)
- Flexible option to use in scripting as well as GUI mode.
- Publication quality plotting, preferably tiled, shifted/multiple X and Y axis, improved legends
- Detailed Tutorials
- Sensible analysis to enable multi-instrument fitting
- Compatible to visualize in all display screens, i.e., desktop, laptop, palmtop etc
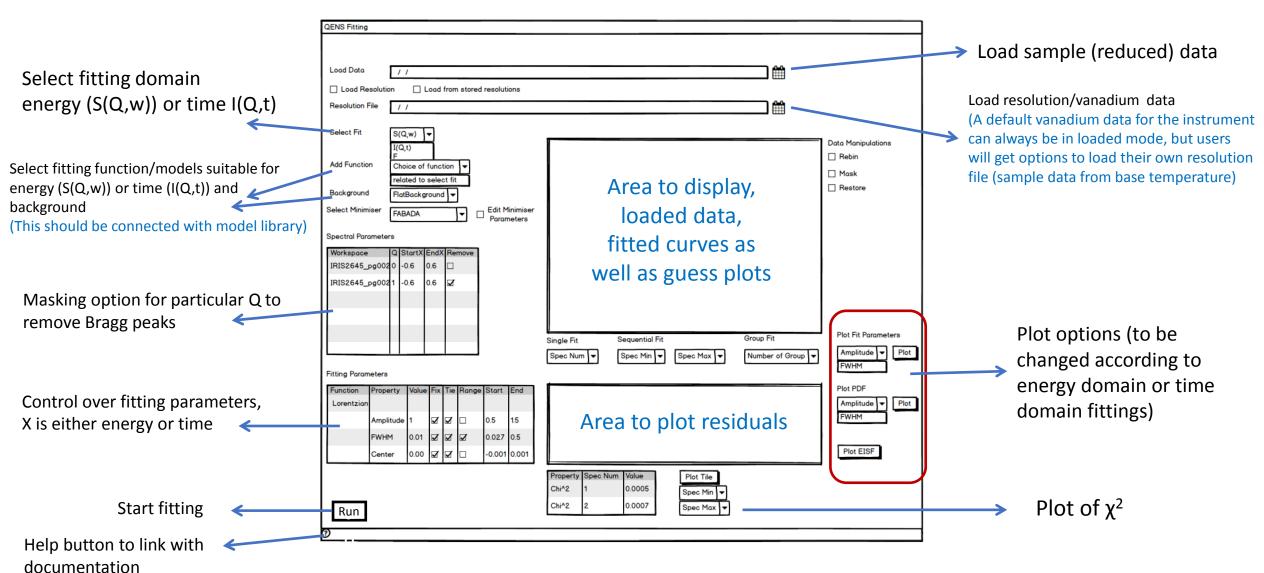
Data reduction related requirements (available before fitting and/or part of QENS fitting interface) :
- Implementation of absorption corrections using various methods.
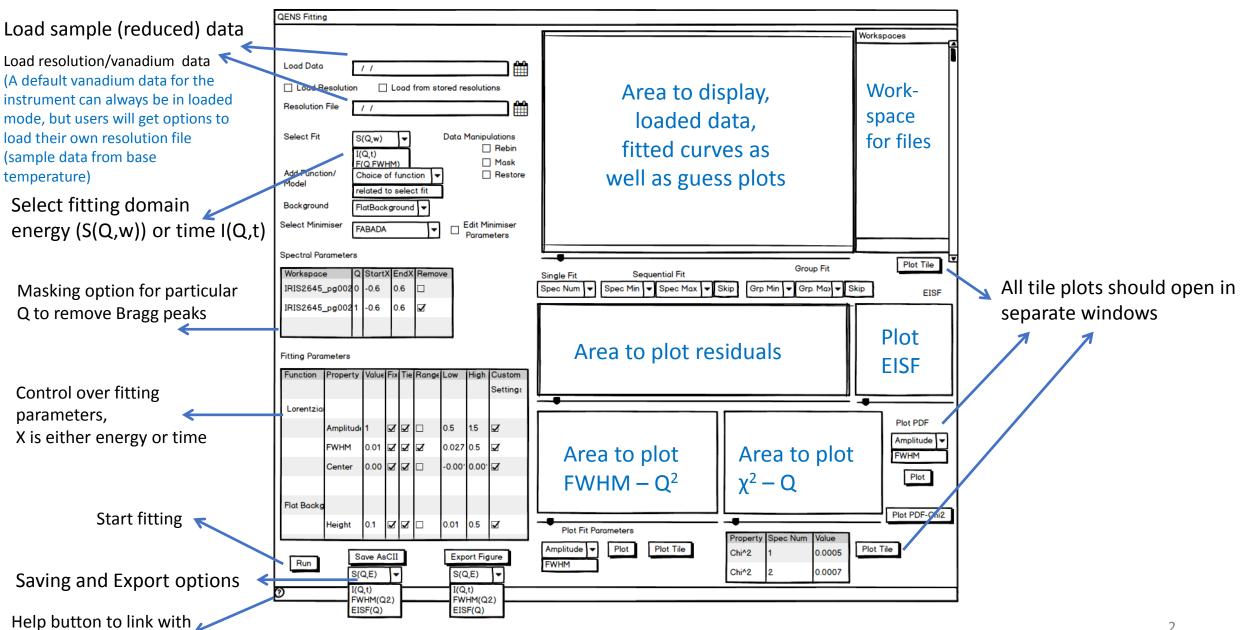- Multiple scattering corrections beyond Mayer's method and Paalman-Pings.

Scope of this GUI will not include but needs further discussion:
- More integration with simulations in data analysis and fitting.

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

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)

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

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

Plot of χ^2

QENS Fitting

Load Data / /

☐ Load Resolution   ☐ Load from stored resolutions

Resolution File / /

Select Fit   S(Q,w) ▼
              I(Q,t)
              F
Add Function Choice of function ▼
              related to select fit
Background   FlatBackground ▼
Select Minimiser FABADA ▼   ☐ Edit Minimiser Parameters

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

Data Manipulations
☐ Rebin
☐ Mask
☐ Restore

Spectral Parameters

Workspace	Q	StartX	EndX	Remove
IRIS2645_pg002	0	-0.6	0.6	☐
IRIS2645_pg002	1	-0.6	0.6	☑

Single Fit   Sequential Fit   Group Fit
Spec Num ▼   Spec Min ▼   Spec Max ▼   Number of Group ▼

Plot Fit Parameters
Amplitude ▼ [Plot]
FWHM

Plot PDF
Amplitude ▼ [Plot]
FWHM

[Plot EISF]

Fitting Parameters

Function	Property	Value	Fix	Tie	Range	Start	End
Lorentzian							
	Amplitude	1	☑	☑	☐	0.5	1.5
	FWHM	0.01	☑	☑	☑	0.027	0.5
	Center	0.00	☑	☑	☐	-0.001	0.001

Area to plot residuals

Property	Spec Num	Value
Chi^2	1	0.0005
Chi^2	2	0.0007

Plot Tile
Spec Min ▼
Spec Max ▼

[Run]

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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

Work-space for files

All tile plots should open in separate windows

Plot EISF

Area to plot residuals

Area to plot FWHM – Q²

Area to plot χ² – Q