

# Mantid Release Presentation

Release 3.4  
ISIS



# What is this meeting

- Release 3.4
  - Released on Monday 18<sup>th</sup> May
  - Present the changes and improvements
- Talk to the team



# Training Courses

- Dates
  - Neutron Training Course
  - Next courses
    - September 2015
    - January 2016



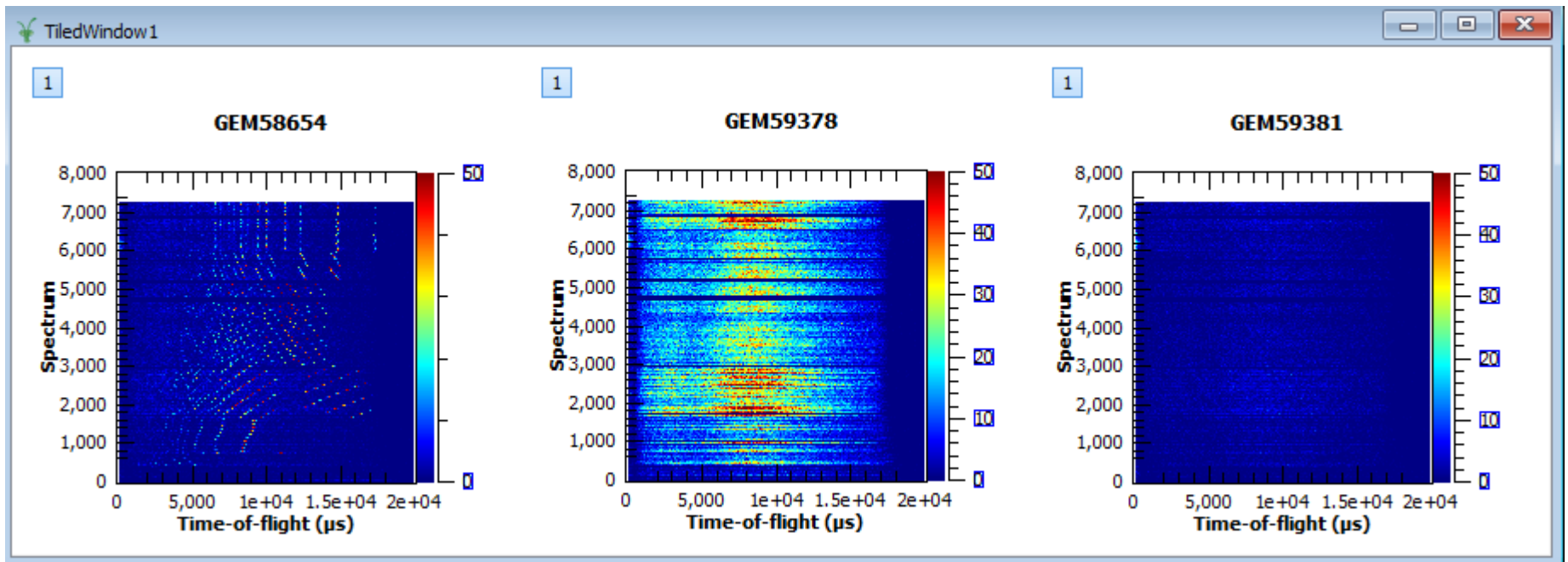
- To Book
  - Email: [nick.draper@stfc.ac.uk](mailto:nick.draper@stfc.ac.uk)
  - More details at [www.mantidproject.org](http://www.mantidproject.org)



# User Interface

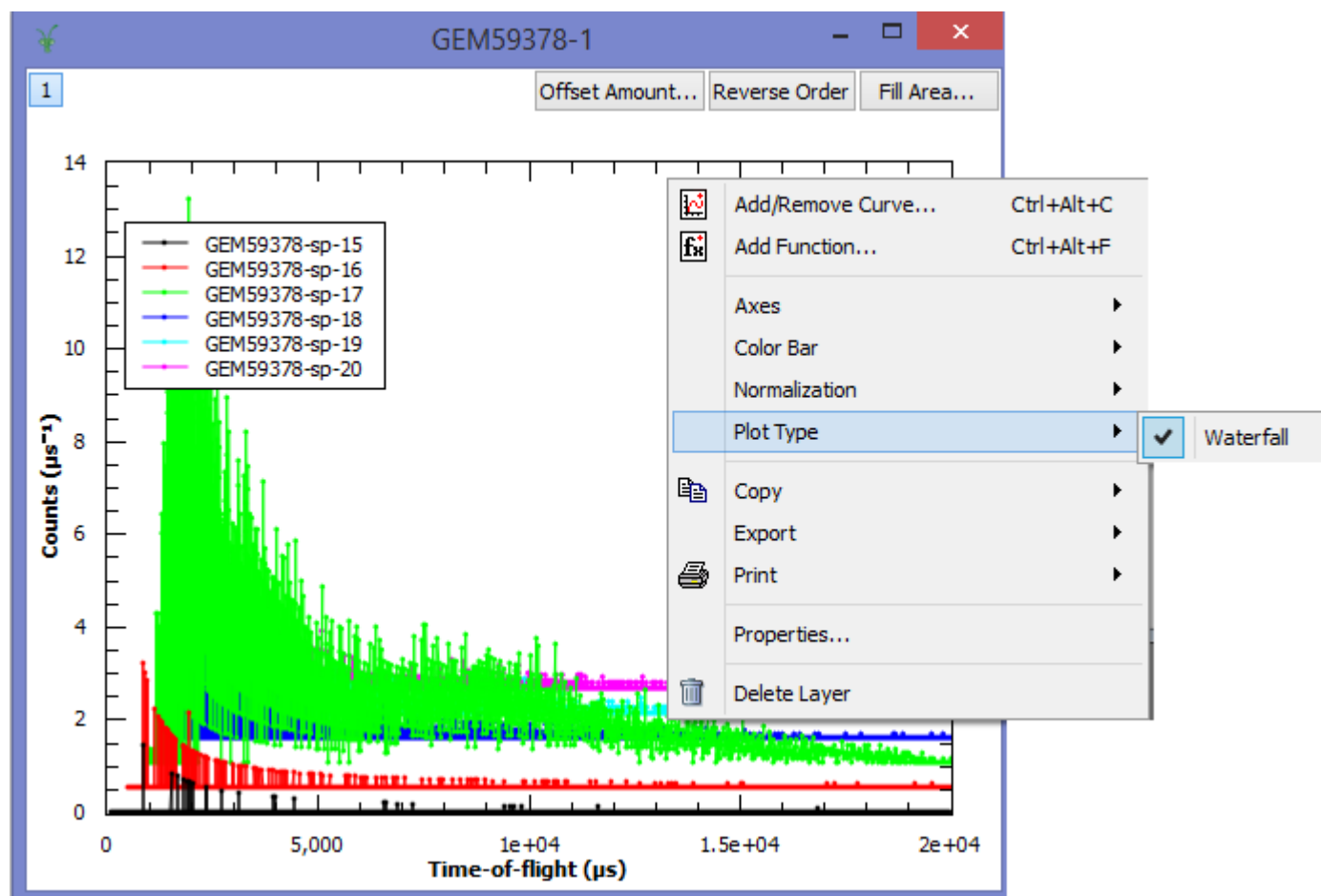


# Tiled Windows



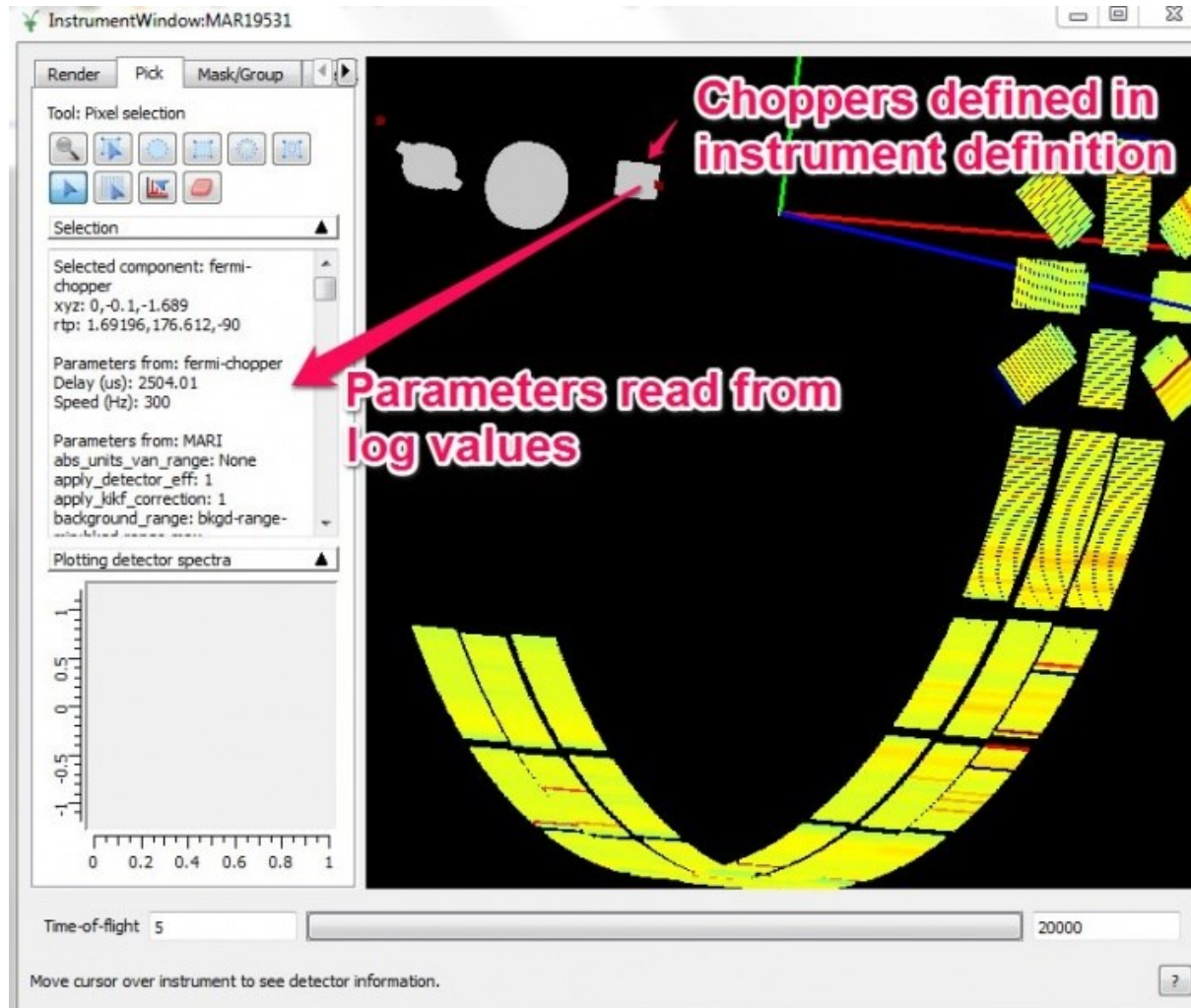


# Water Fall Plots



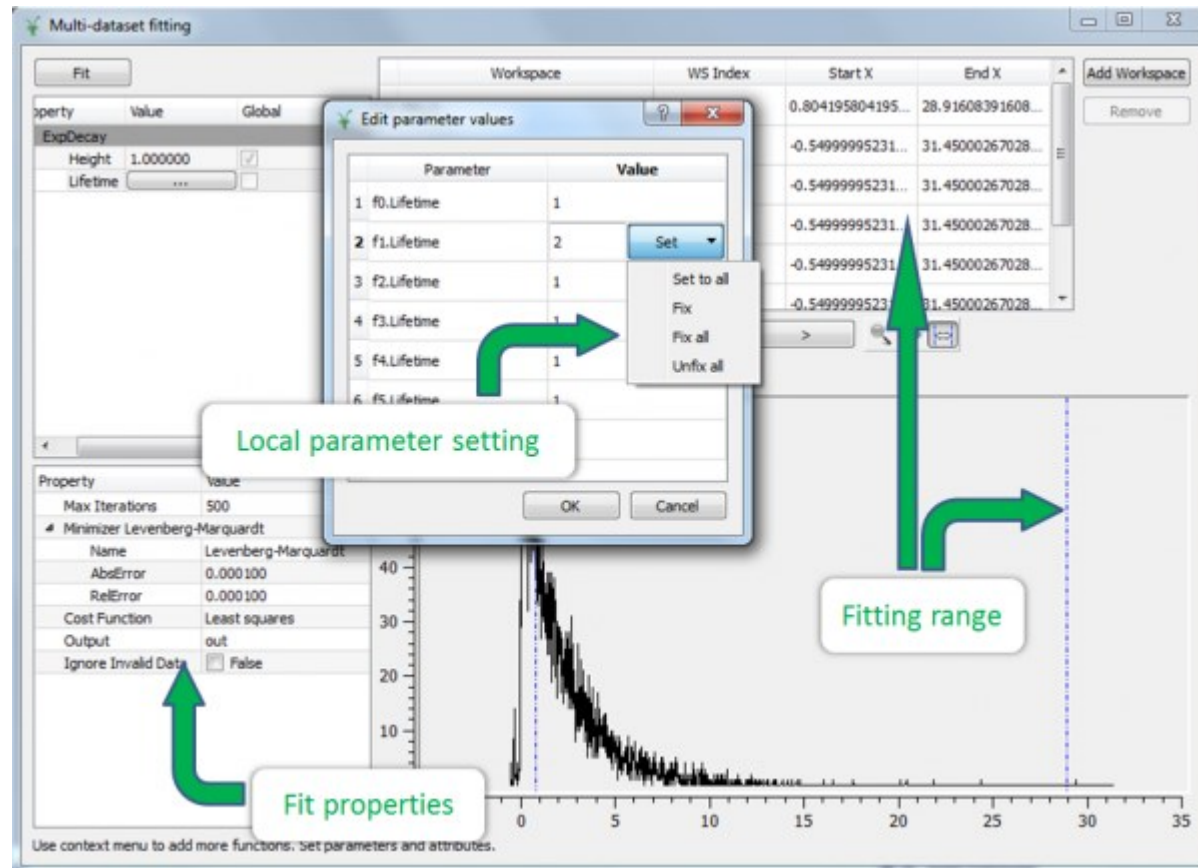


# Non-detector Components





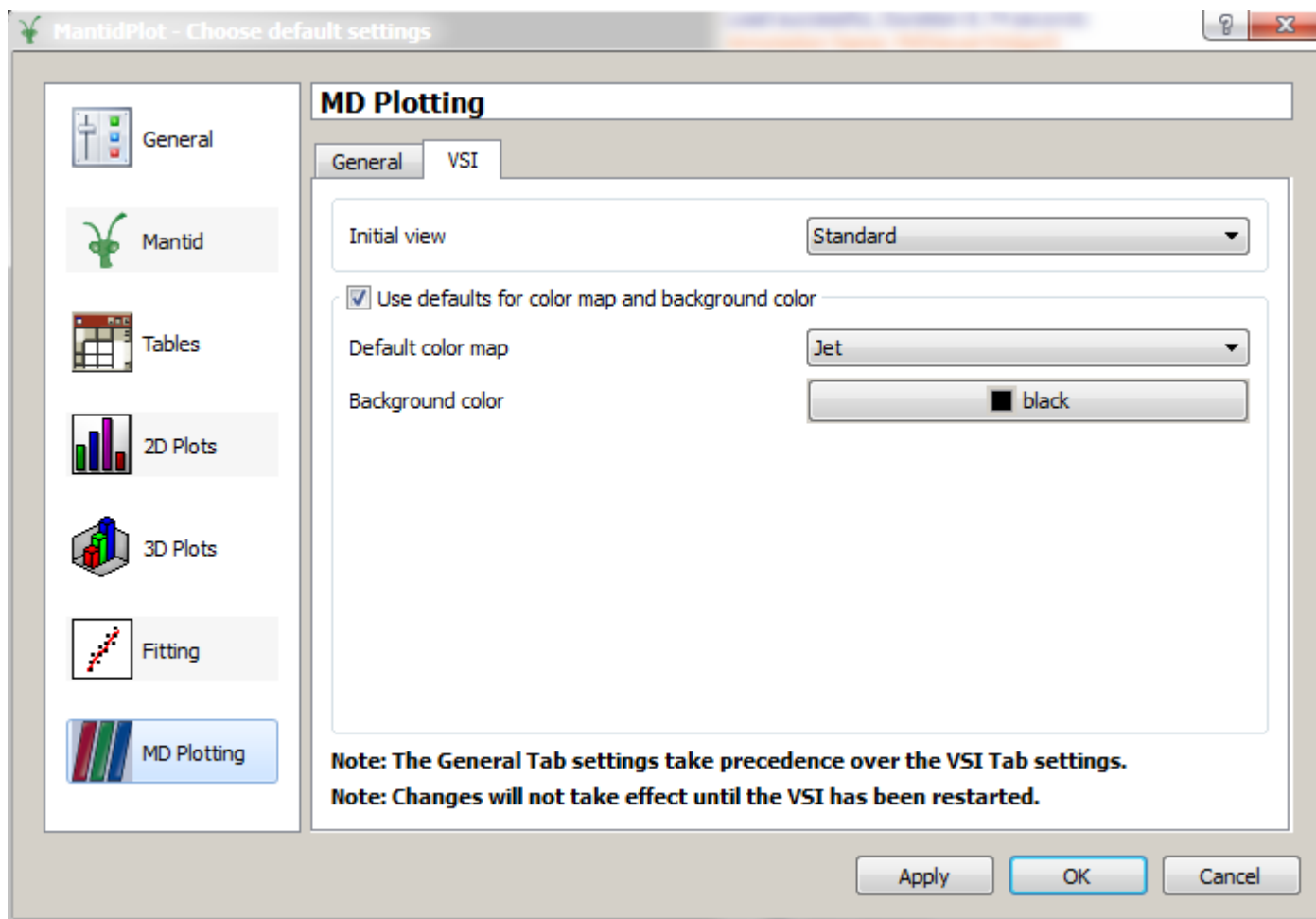
# Multi-data Fitting





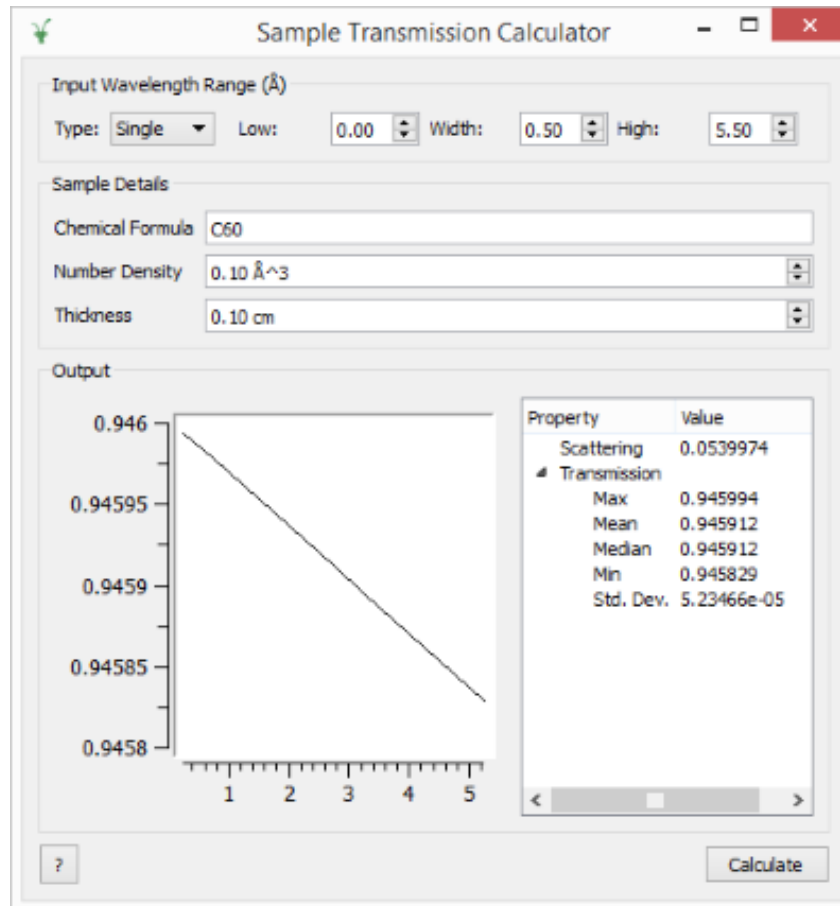


# MD Viewer (VSI)





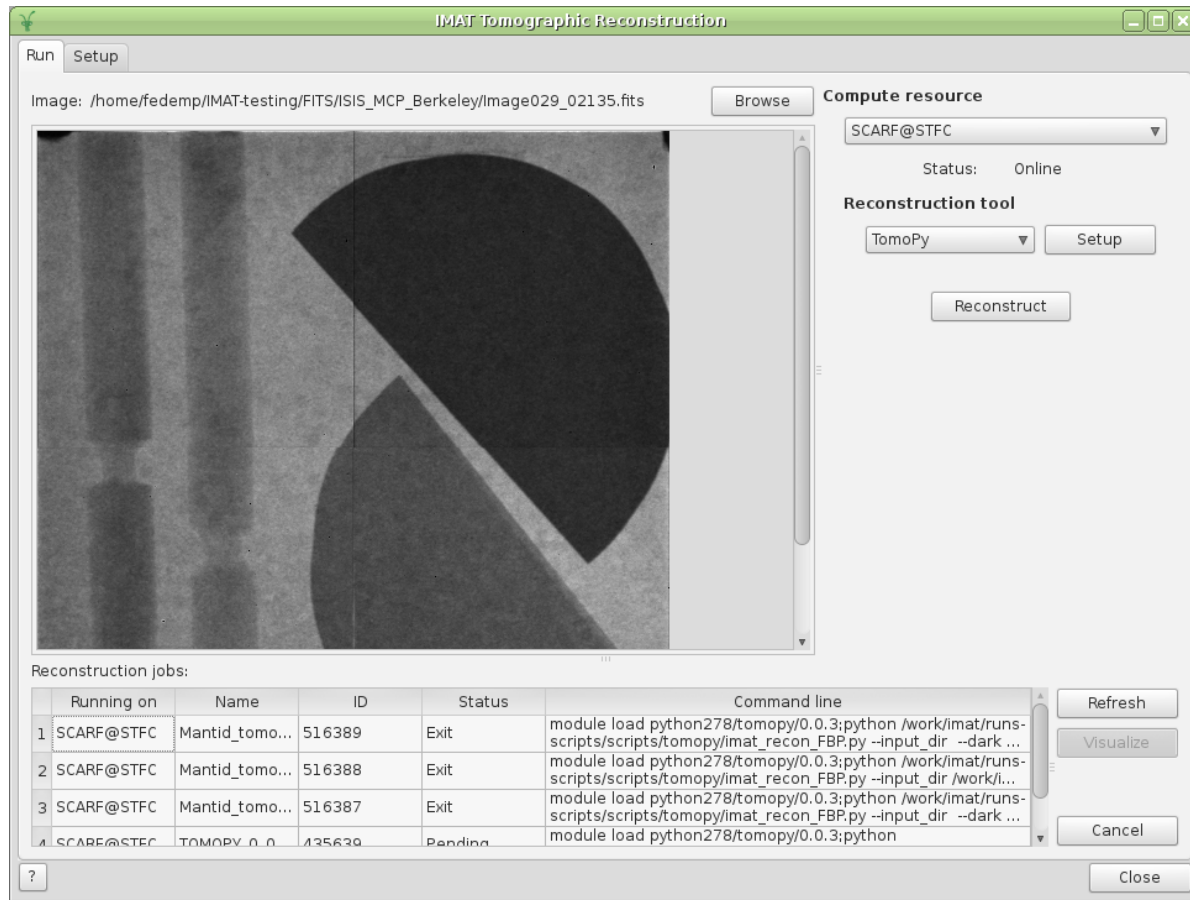
# New Sample Transmission Calculator





# Other Important Changes

- Tomographic Reconstruction User Interface
- **SliceViewer, LineViewer and PeaksViewer**





# Framework



# Framework – Improvements

- ParaView bundled with the installation packages



- Instrument definitions
  - LET, ALF and others at SNS updated
  - You get these updates automatically since v3.3

- Infrastructure for distributed computing

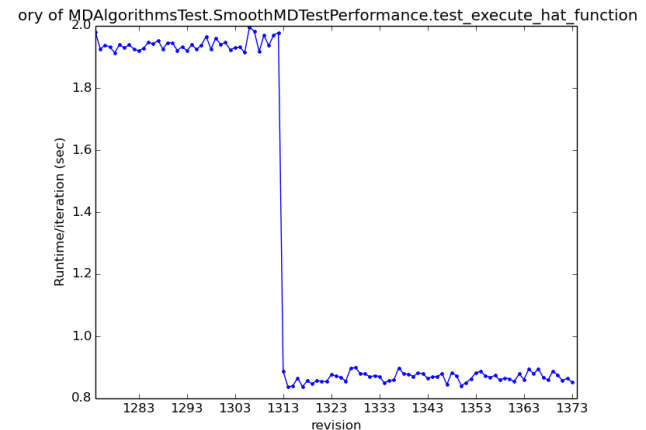
- Algorithms:
  - ~40 new ones
  - ~100 improved/extended





# Performance Improvements

- MergeMDFiles – Manages memory more efficiently, improving performance up to 30%
- MergeMD – Only loads experiment information when needed, can save hours in a large MergeMD run
- SaveNXSPE – Writes to disk more efficiently
  - Runs 2x faster
  - Now saves to CEPH quickly
- LoadNexusProcessed loads multi-period workspaces more efficiently, up to 100x faster
- Project saving places multiperiod data in a single Nexus file now, which is approximately 5x faster
- SmoothMD and some other multi-dimensional algorithms are running 2x faster than they were during testing

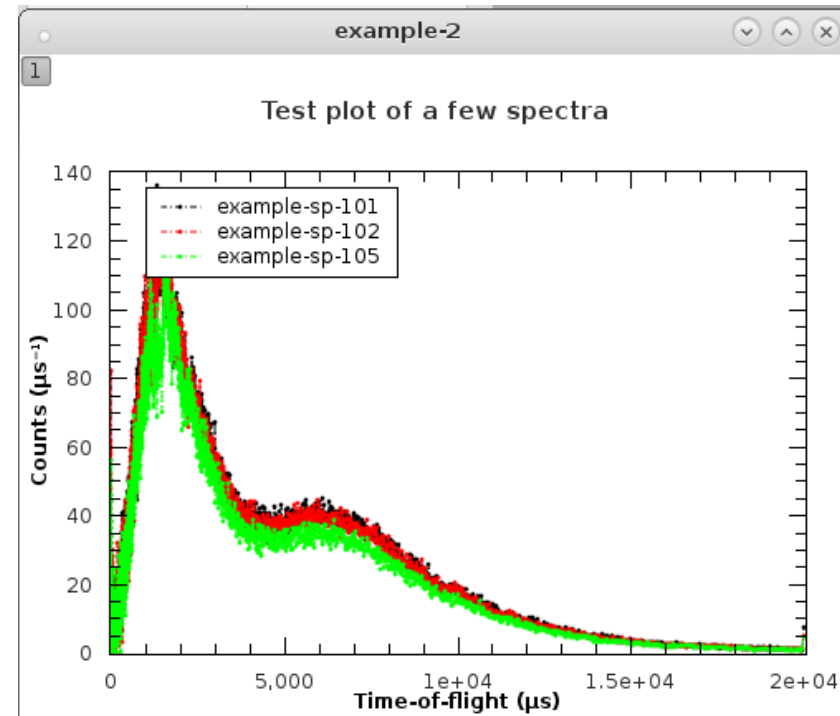


# Python Plotting Command Line Interface

- New Python plotting interface now available by default. Like:
  - Python matplotlib
  - Matlab plot commands
- Interface:
  - Supports: plotSpectrum / Bin / MD
  - Interface:
    - Functional
    - Object-oriented
  - *kwargs*: `linestyle='-.'`, `color='red'`
  - VSI planned – feedback welcome
- Not to be confused:
  - Matplotlib - also **shipped**

**(import matplotlib)**

**MANTID**



```
In [26]: example = Load("MAR1060.raw", OutputWorkspace="example")
```

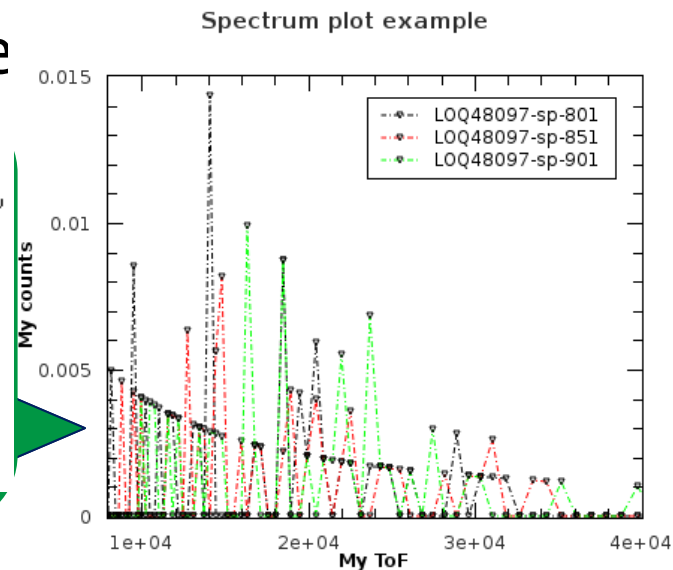
```
In [27]: lines = plot(example, [100, 101, 104], linestyle='-.')
```

```
In [28]: title('Test plot of a few spectra')
```

# Python Plotting Command Line Interface

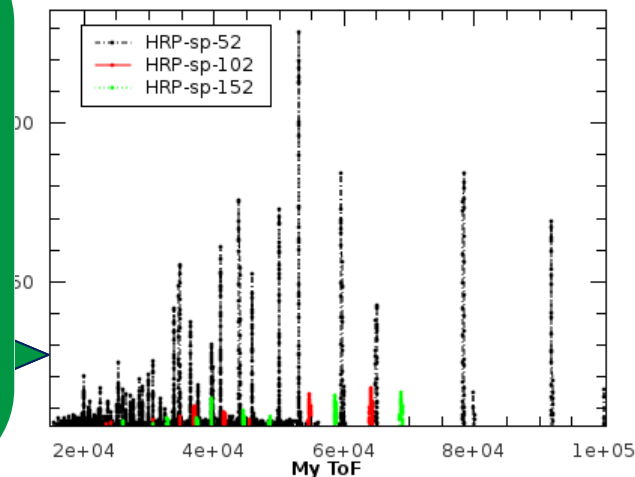
- Plotting spectra, functional interface

```
loq=Load('LOQ48097.raw', OutputWorkspace="LOQ48097")
plot(loq, [800, 850, 900], linestyle='-.', marker='v',
      linewidth=1)
title('Spectrum plot example')
ylabel('My counts')
xlabel('My ToF')
xlim(8000, 4e4)
ylim(0, 0.015)
```



- Object-oriented interface (Figure, Axis, Line2D, etc.):

Spectrum plot example - HRP







# Python Plotting Command Line Interface

- To learn how to use it:
  - `help(pymantidplot.pyplot)`
  - <http://docs.mantidproject.org/nightly/api/python/index.html>
  - Familiar interface, >90% like the Pyplot tutorial:  
[http://matplotlib.org/users/pyplot\\_tutorial.html](http://matplotlib.org/users/pyplot_tutorial.html)

The screenshot shows the Mantid project's documentation website. A green line starts from the third bullet point in the list above, curves around the left side of the page, and points to the 'Scripting' section under 'Mantid Training Courses'. A blue oval highlights the text 'Courses Sep/Jan' with a blue arrow pointing to the 'Mantid Training Courses' section. The 'Scripting' section is also circled in green.

**MANTiD**

Home Downloads Documentation Develop Contact Us Search

## Documentation [edit]

Online Help Pages [edit]

### Installation [edit]

- System Requirements
- Packages [link], along with install instructions for supported environments
- Operating system specific issues

### Usage [edit]

- Examples of Mantid Usage
- Concepts
- Mantidplot Help
- Algorithm Descriptions [link]
- Fit Functions [link]

### Mantid Training Courses [edit]

- Mantid Introduction
- Introduction to Python
- Python and Mantid
- Extending Mantid with Python

### Scripting [edit]

- Python API reference (searchable help) [link]
- Learning Python
- Introduction to numpy [link]
- Mantid Python without MantidPlot
- Using Mantid with IPython Notebook

### Extending Mantid [edit]

- Write your own algorithm
- Create a customized input dialog
- Doxygen code documentation [link]
- Develop
- Algorithms used in testing and validation

### Instrument/Technique Specific Mantid Documentation [edit]

- Scientific Techniques
- VATES



# Indirect Inelastic



# Absorption Corrections

- Added cross platform absorption correction algorithms based on those already in MANTID
- New tab on Indirect Data Analysis to provide a simplified interface to the algorithms

The screenshot shows the 'Indirect Data Analysis' window with the 'Absorption Corrections' tab selected. The interface is organized into several sections:

- Input:** Contains 'Sample Input' and 'Use Container' fields, each with a 'File' dropdown and a 'Browse' button.
- Shape Details:** Includes a 'Shape' dropdown set to 'Flat Plate', and input fields for 'Sample Width', 'Sample Height', 'Sample Thickness', 'Container Front Thickness', 'Container Back Thickness', and 'Element Size', all with numerical values and up/down arrows.
- Sample Details:** Features 'Number Density' (0.10000 A<sup>-3</sup>) and 'Chemical Formula' (empty) fields.
- Container Details:** Includes a 'Use Container Corrections' checkbox, a 'Scale' field (0.00000), and another 'Number Density' and 'Chemical Formula' pair.
- Output Options:** Contains checkboxes for 'Keep Correction Factors', 'Plot Result', and 'Save Result'.

At the bottom, there are buttons for '?', 'Py', 'Run', and 'Manage Directories'.



# Absorption Corrections

- ❑ Major refactor of old absorption correction routines
- ❑ In preparation of porting cylinder absorption routine from FORTRAN
- ❑ Updates to the Calculate and Apply Corrections interfaces

The screenshot shows the 'Indirect Data Analysis' software window with the 'Absorption Corrections' tab selected. The interface is organized into several sections:

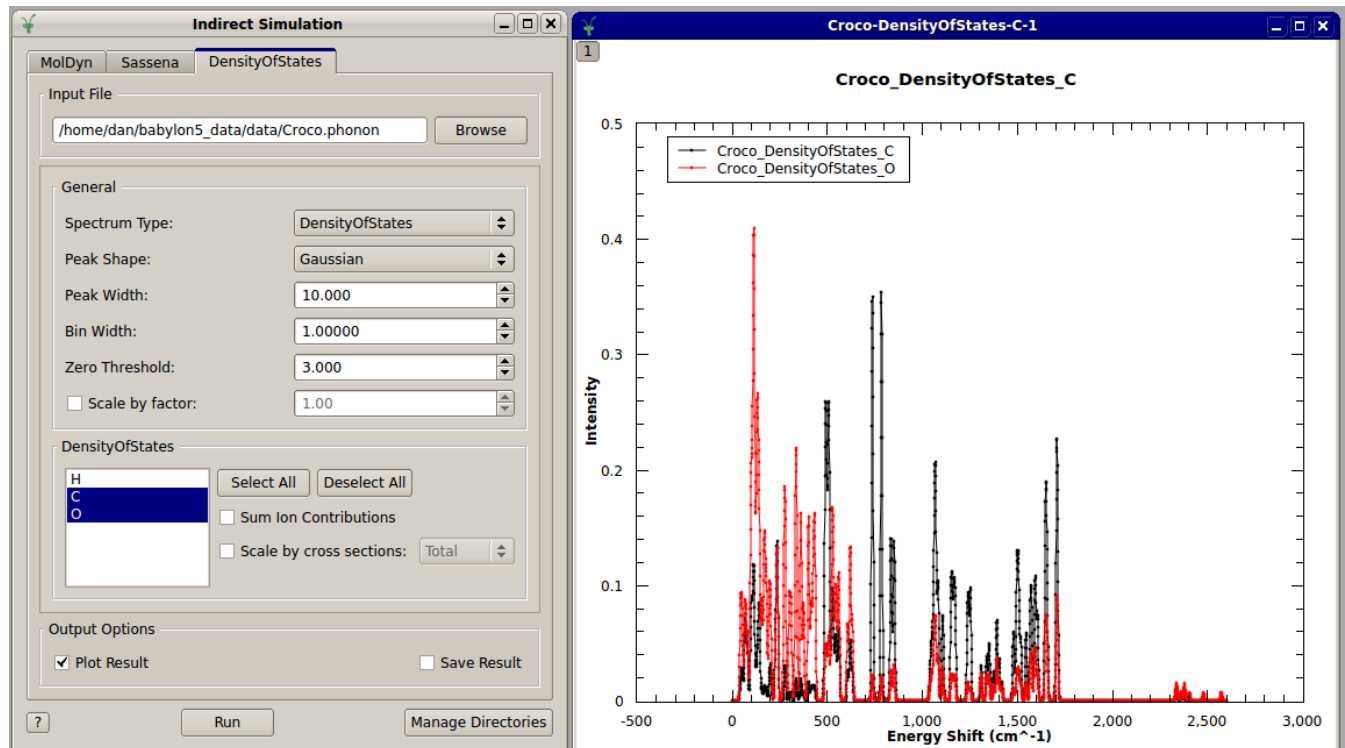
- Input:** Contains 'Input type' (set to 'File') and 'Use Can' (unchecked) options, each with a text field and a 'Browse' button.
- Shape Details:** Includes 'Sample Shape' (set to 'Flat Plate'), 'Sample Thickness' (0.000 cm), 'Sample Angle' (0.000), 'Container Front Thickness' (0.000 cm), and 'Container Back Thickness' (0.000 cm).
- Sample Details:** Includes 'Number Density' (0.00) and 'Chemical Formula' (empty).
- Can Details:** Includes 'Number Density' (0.00) and 'Chemical Formula' (empty).
- Output Options:** Includes 'Plot Output' (set to 'None') and a 'Save Result' checkbox.

At the bottom of the window, there are buttons for '?', 'Py', 'Run', and 'Manage Directories'.



# Interface Updates

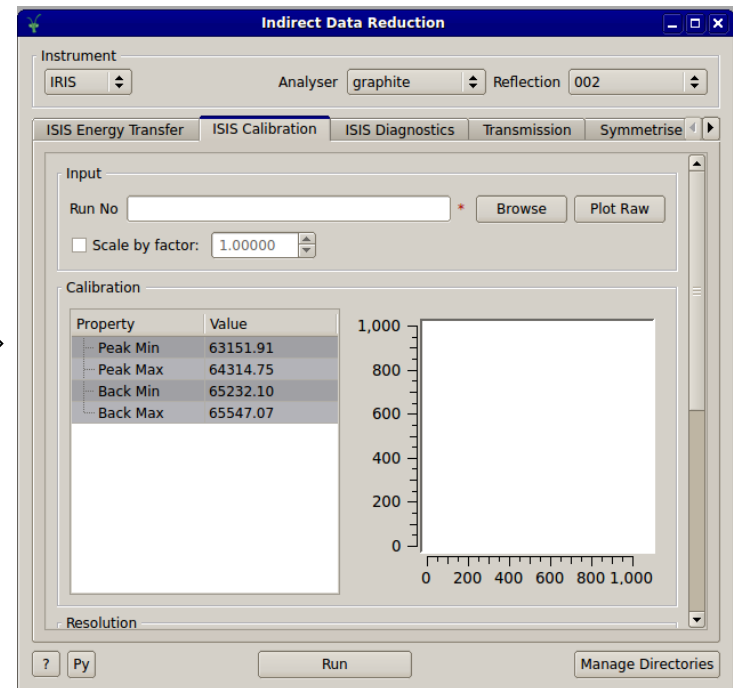
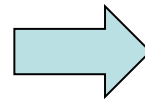
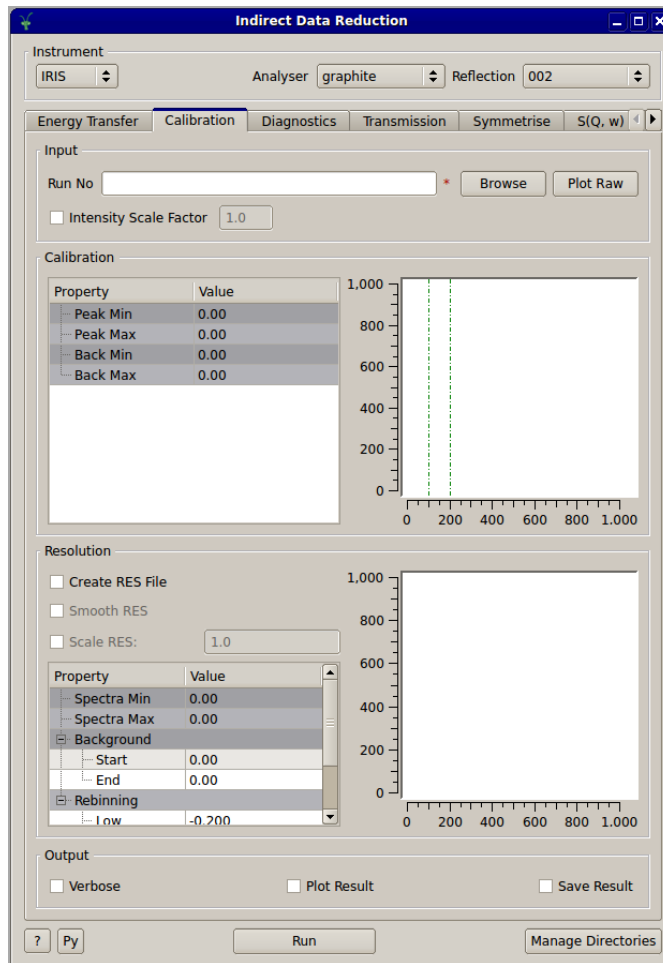
- ❑ Added DensityOfStates tab to Indirect Simulation interface
- ❑ Allows easier selection of a partial DOS from CASTEP output





# Interface Updates

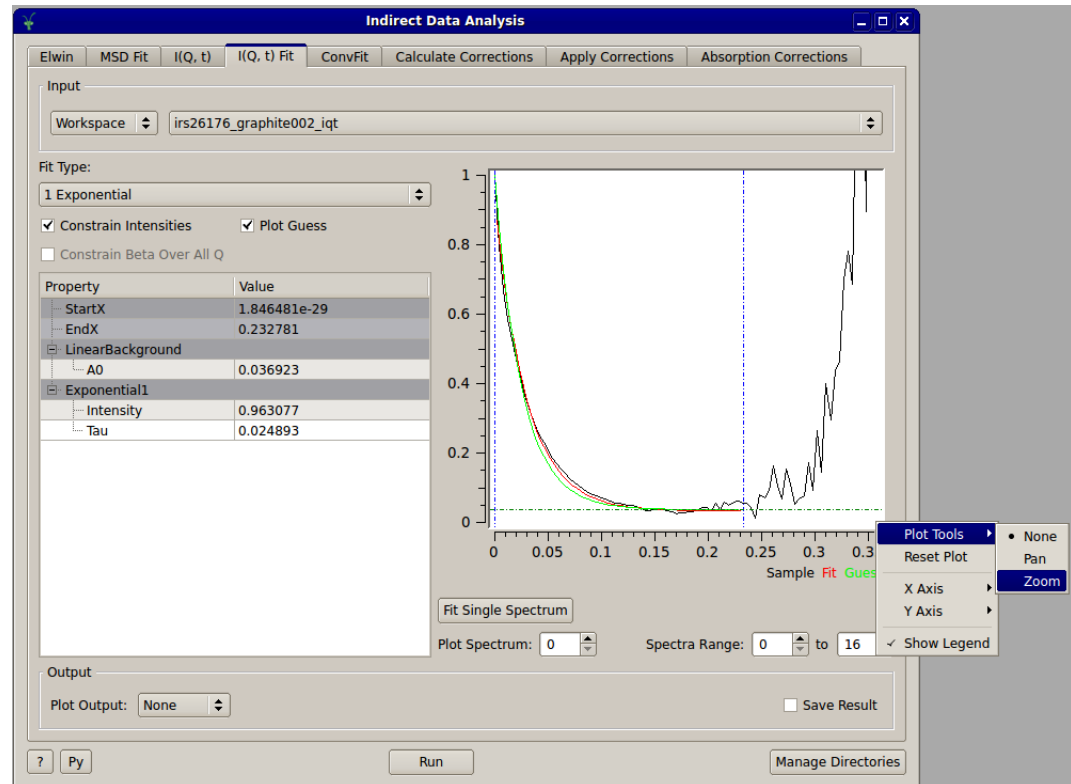
- ❑ Various indirect interfaces modified to be usable on low resolution displays





# Interface Updates

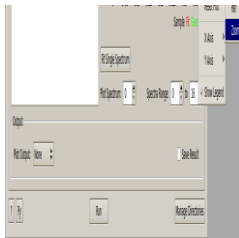
- ☐ Standard preview plot widget in all indirect interfaces
- ☐ Supports:
  - ☐ Changing axis scales
  - ☐ Pan tool
  - ☐ Zoom tool
  - ☐ Automatic zooming
  - ☐ Legend toggle





# Interface Documentation

- ❑ Added offline documentation for all indirect user interfaces
- ❑ Accessible from ? Button in bottom left of interface window



Similarly to FuryFit, ConvFit provides a simplified interface for controlling various fitting functions (see the [Fit](#) algorithm for more info). The functions are also available via the fit wizard.

Additionally, in the bottom-right of the interface there are options for doing a sequential fit. This is where the program loops through each spectrum in the input workspace, using the fitted values from the previous spectrum as input values for fitting the next. This is done by means of the [PlotPeakByLogValue](#) algorithm.

A sequential fit is run by clicking the Run button at the bottom of the tab, a single fit can be done using the Fit Single Spectrum button underneath the preview plot.

### Fitting Model

The model used to perform fitting is described in the following tree, note that everything under the Model section is optional and determined by the *Fit Type* and *Use Delta Function* options in the interface.

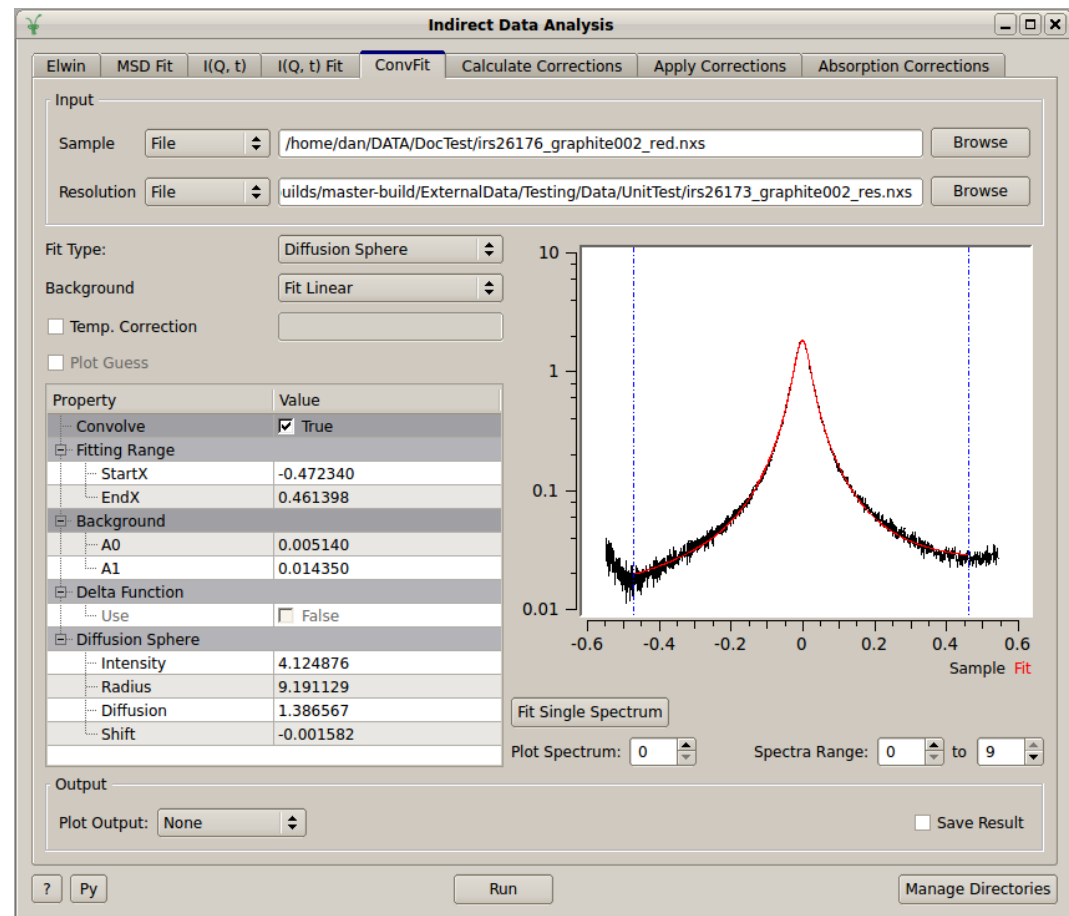
- [CompositeFunction](#)
  - [LinearBackground](#)
  - [Convolution](#)
    - Resolution
    - Model ([CompositeFunction](#))
      - [DeltaFunction](#)
      - [ProductFunction](#)
        - [Lorentzian](#)
        - Temperature Correction
      - [ProductFunction](#)
        - [Lorentzian](#)





# ConvFit

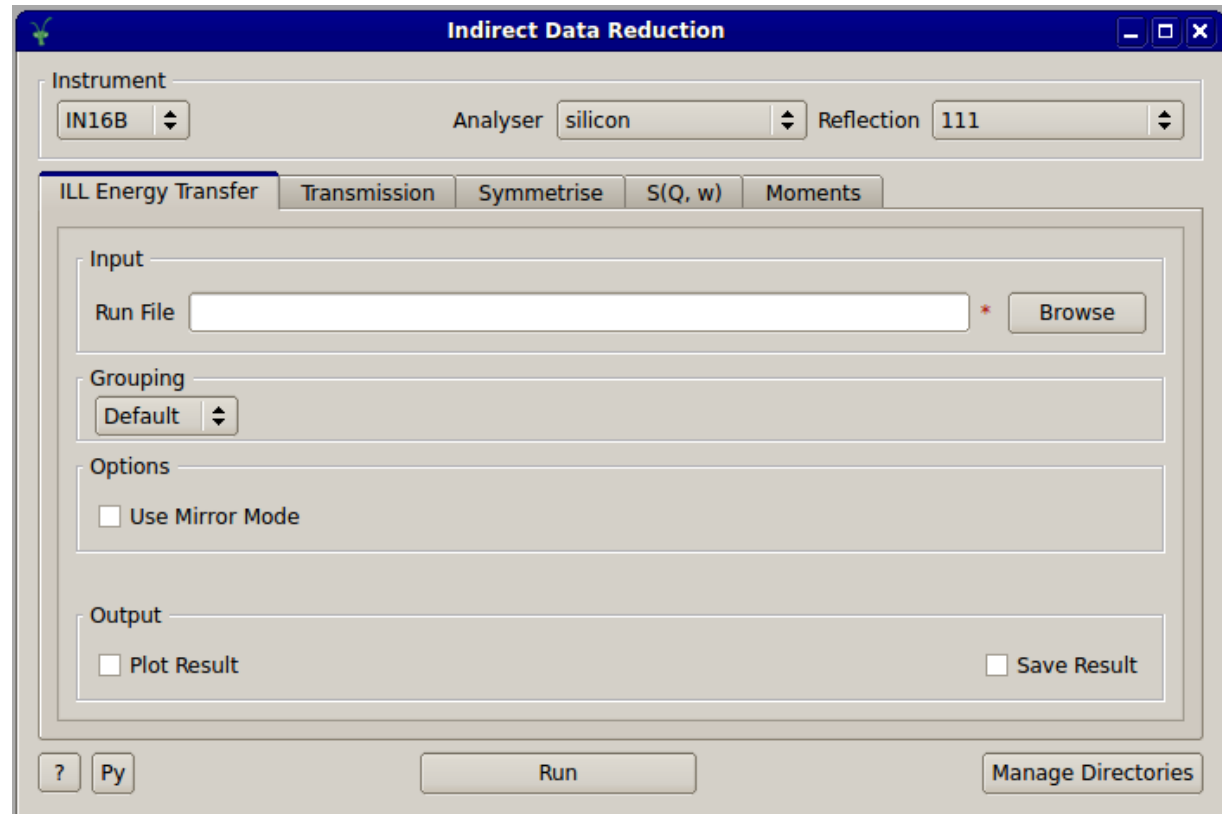
□ Add support for DiffSphere and DiffRotDiscreteCircle to IDA ConvFit interface





# IDR Multiple Facility Support

- ❑ Added support for IN16B reduction on Indirect Data Reduction
- ❑ Allow entire UI to be customised per facility





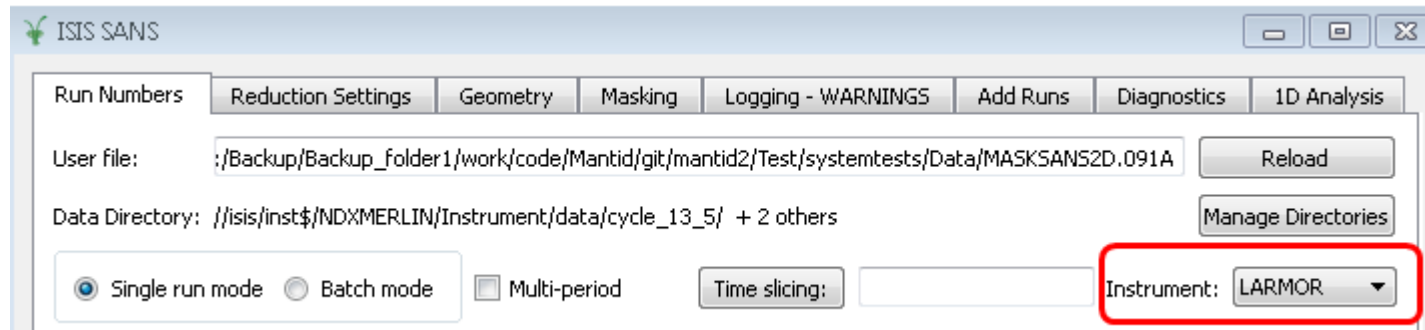
SANS



# SANS

## ISIS SANS GUI

- Support for LARMOR



- Allow added event files to be reduced !

## SasView

- Overhaul of documentation
- New models added

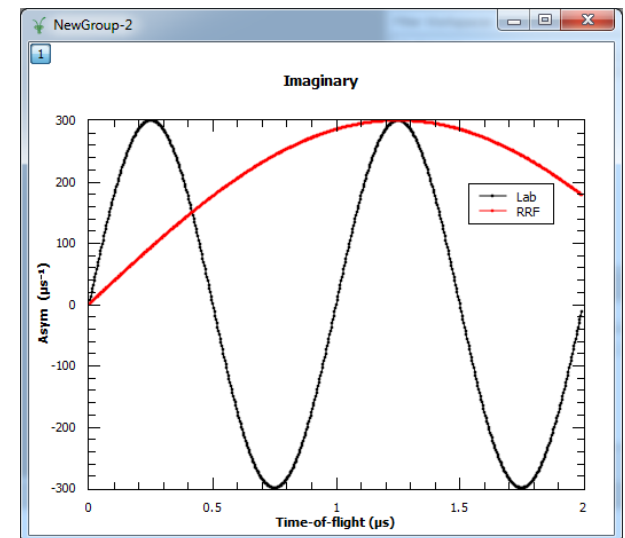
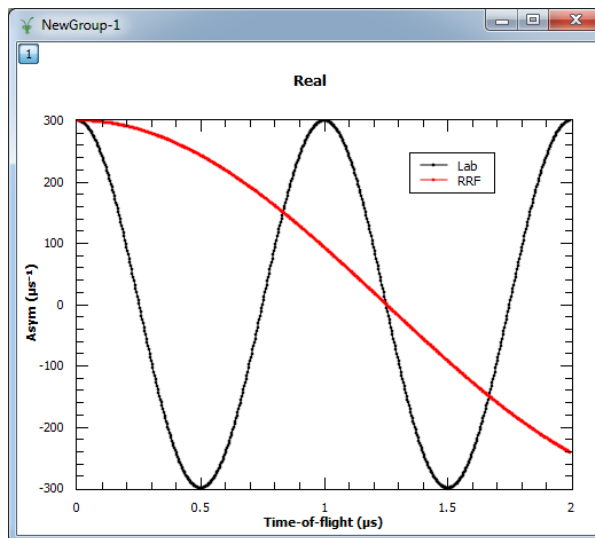
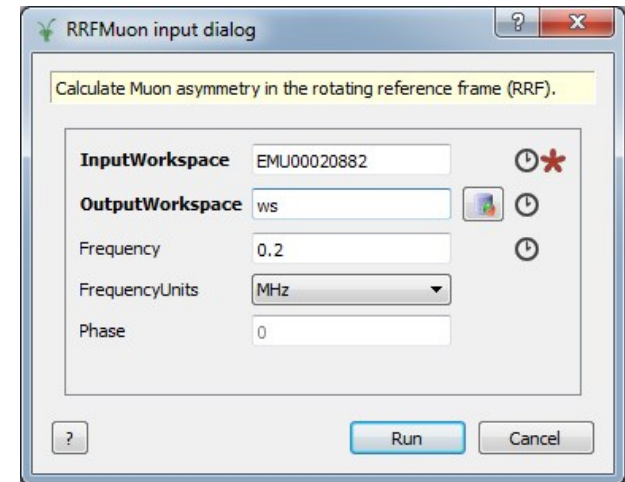


# Muon



# New RRFMuon algorithm

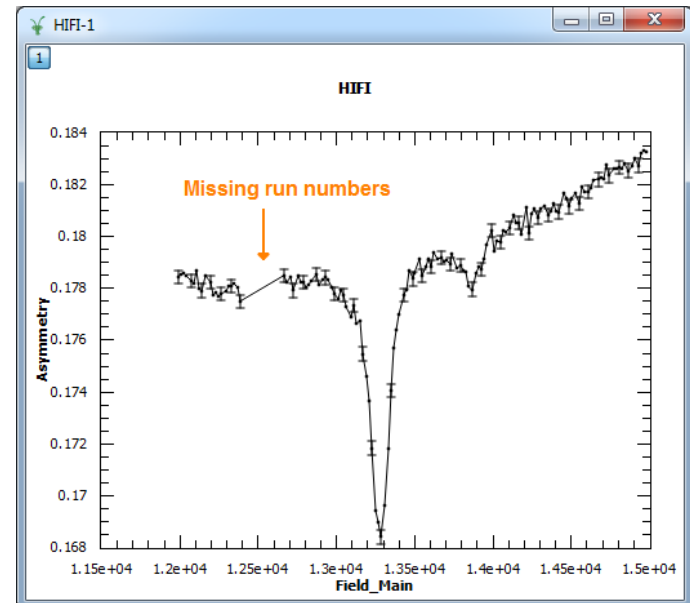
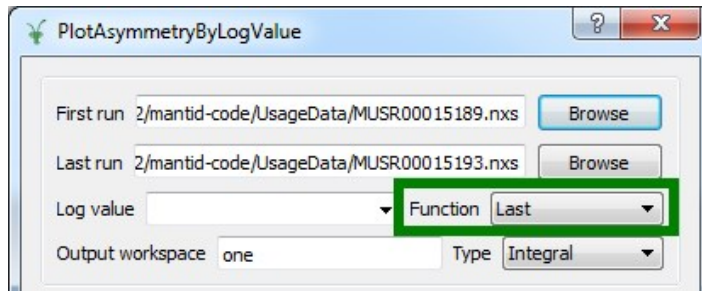
- Real + Imag part of a signal
- Frequency units:
  - MHz
  - Gauss
  - Mrad/s





# Existing algorithms

- LoadMuonNexus
  - Correct labelling of specified spectra (Min/Max/List)
  - DeadTimeTable and DetectorGroupingTable containing specified spectra only
- PlotAsymmetryByLogValue
  - Missing run numbers are allowed
  - Functions of LogValue: Mean, Min, Max, First, Last

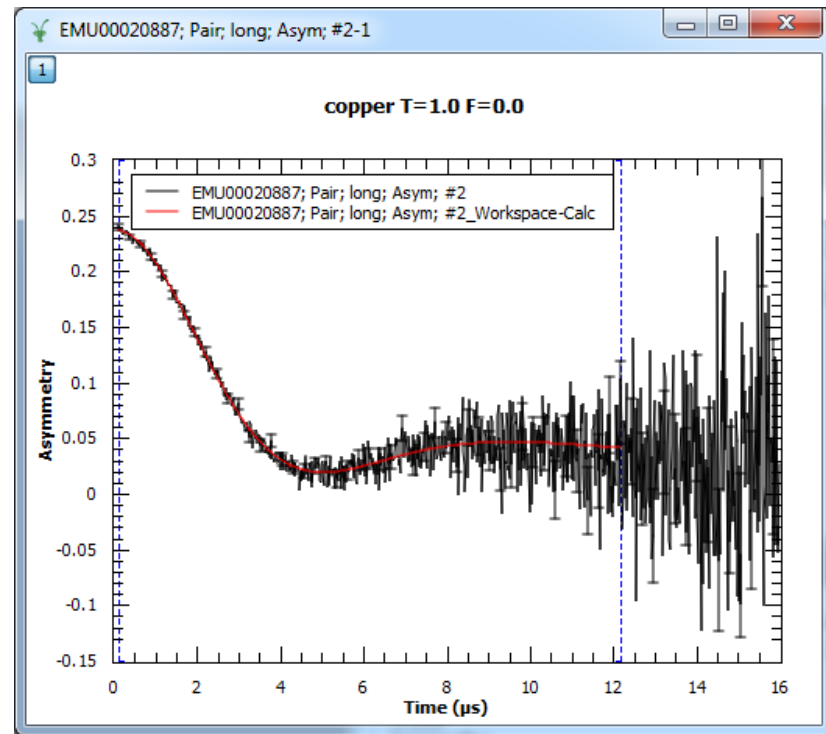




# DynamicKuboToyabe fitting function

$$G_Z(t) = g_Z(t)e^{-\nu t} + \nu \int_0^t g_Z(\tau)e^{-\nu\tau} G_Z(t - \tau)d\tau$$

- Muon category
- Fitting parameters:
  - Asymmetry A
  - Local field  $\Delta$
  - External field F
  - Hopping rate  $\nu$
- Attribute:
  - Bin width

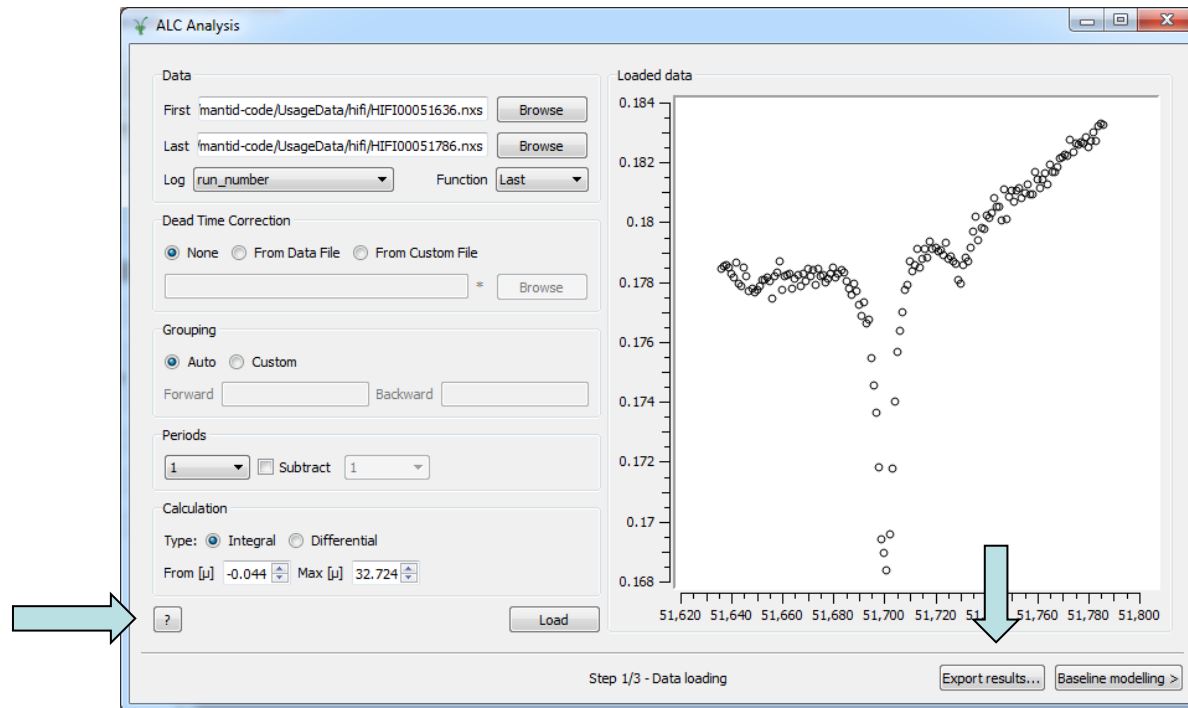




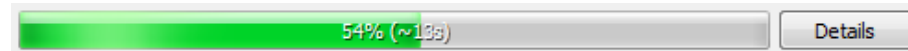


# ALC Interface

- Help buttons “?” & “Export results...”



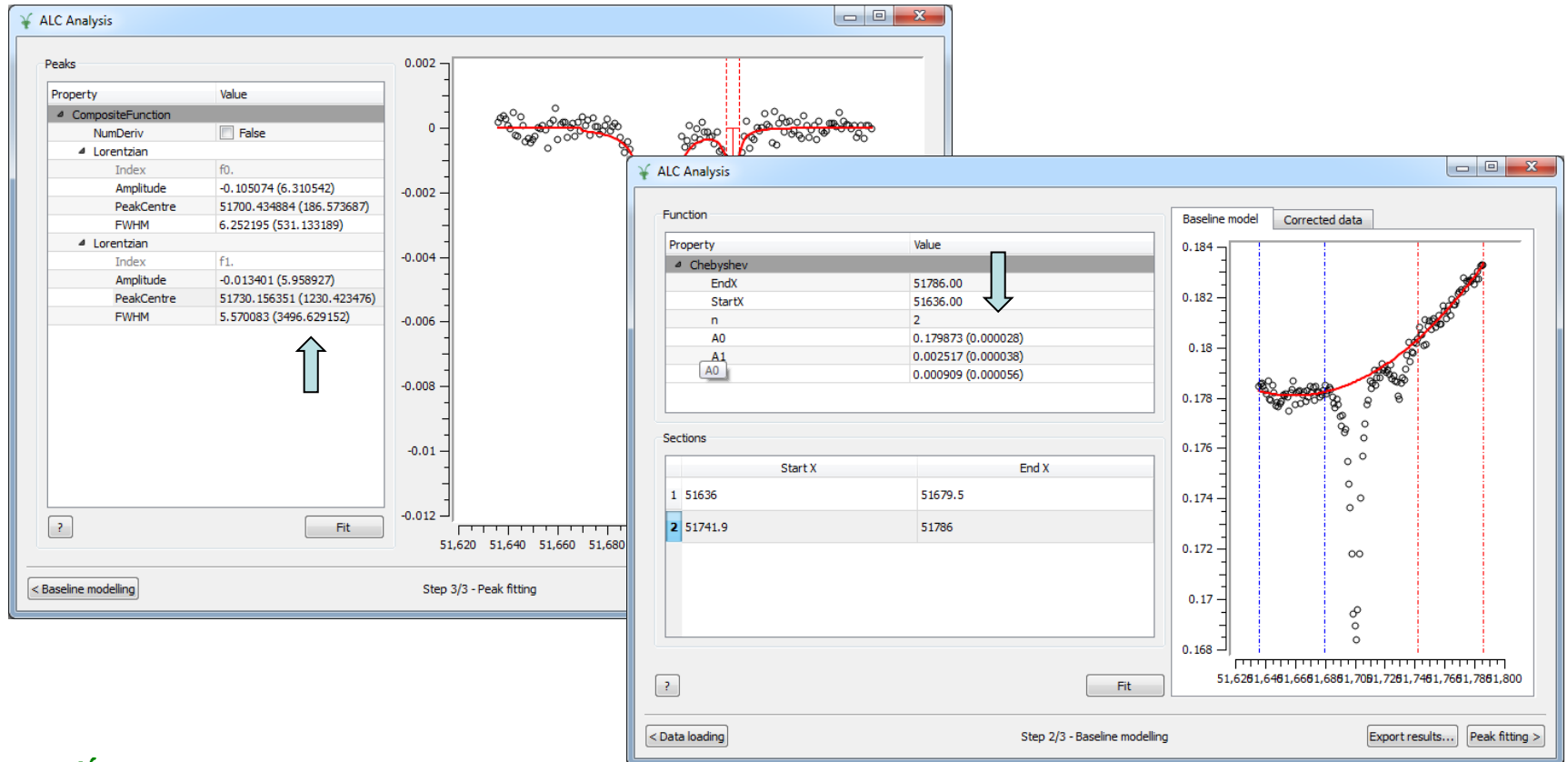
- DataLoading:
  - Progress bar
  - Missing options added





# ALC Interface

- Parameter errors
- BaselineModelling: range selectors



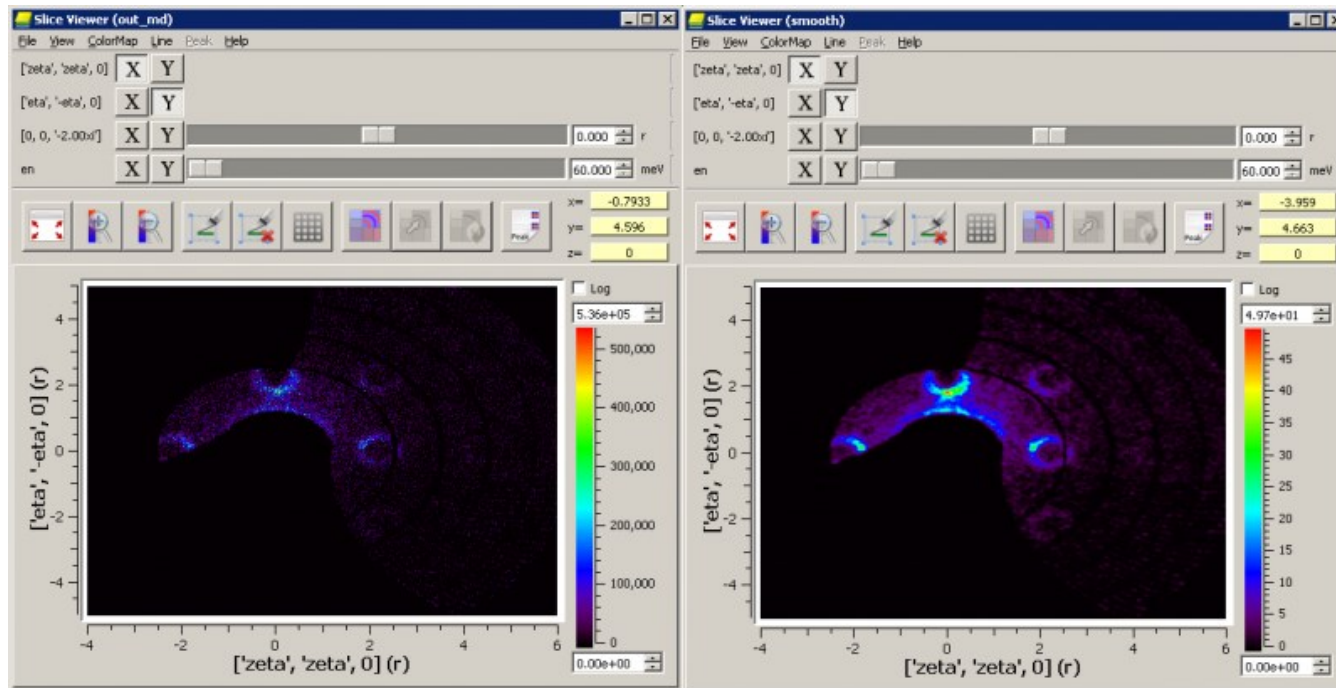


# Direct Inelastic



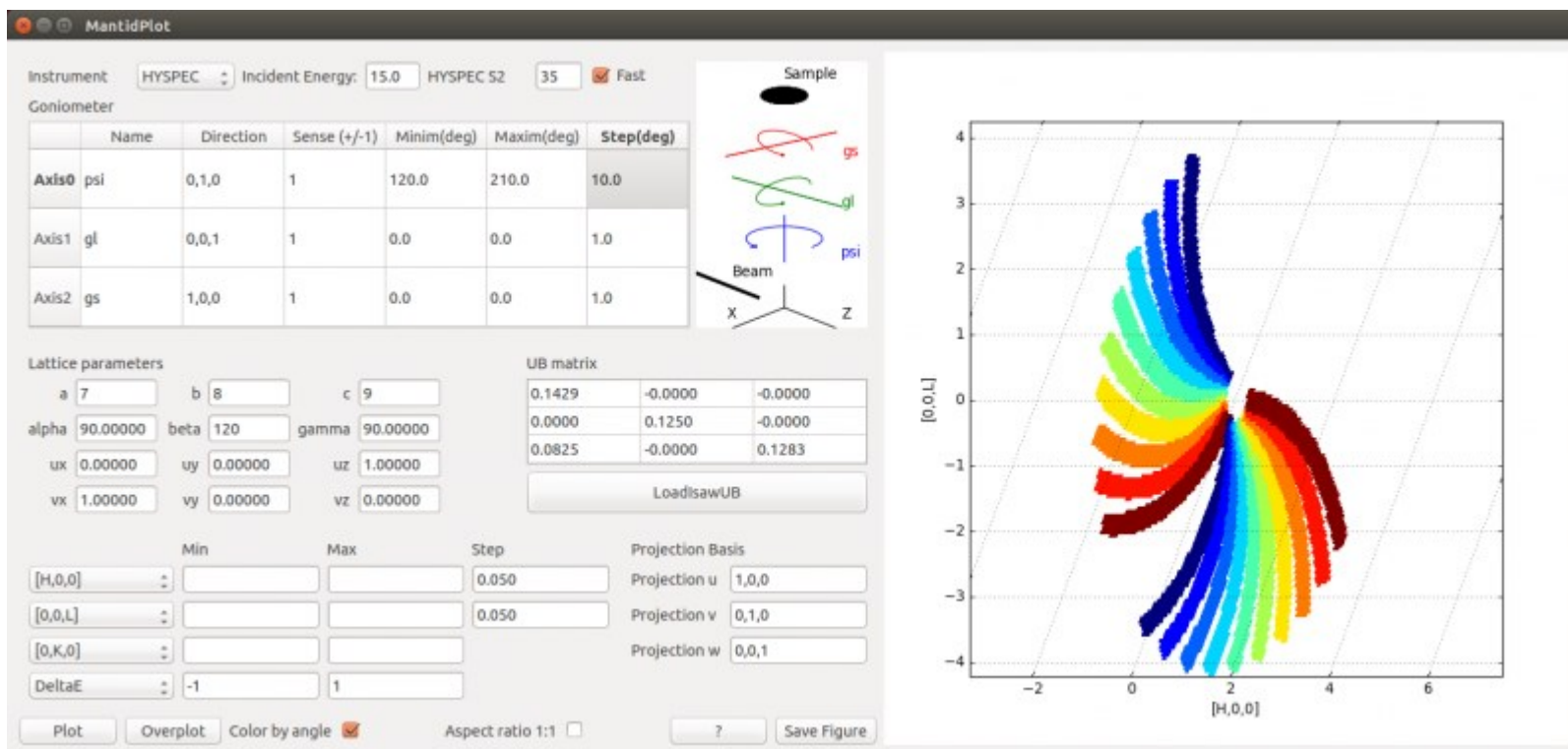
# Horace Style Commands

- **CutMD** equivalent to **cut\_sqw**
  - Introduction of Horace style Projections into Mantid
- **CreateMD** equivalent to **gen\_sqw**
  - Creates merged workspaces in one step
  - With a file-backed mode
- **SmoothMD** equivalent to **smooth**
- **IntegrateMDHistoWorkspace**



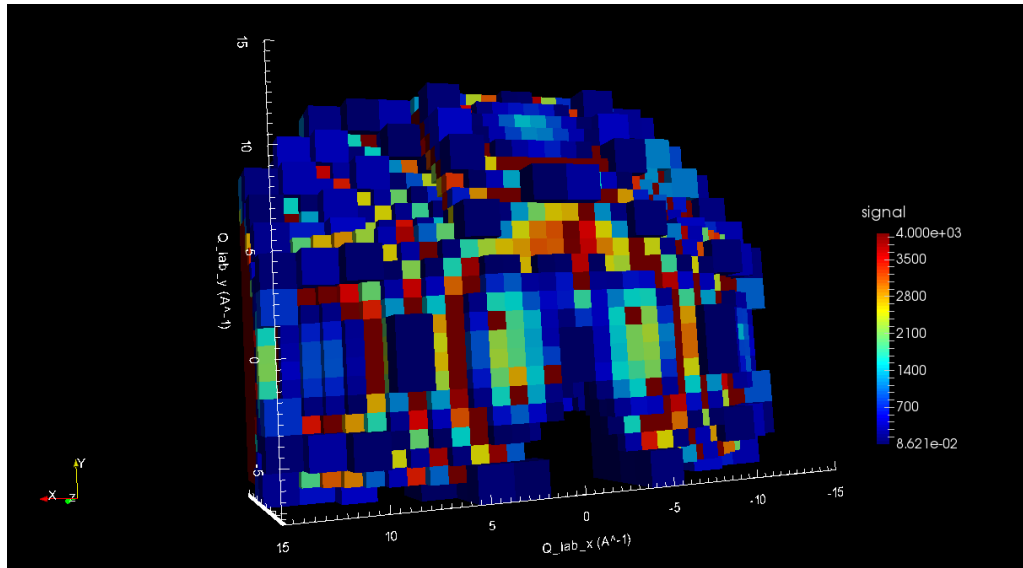


# New DGS Planner





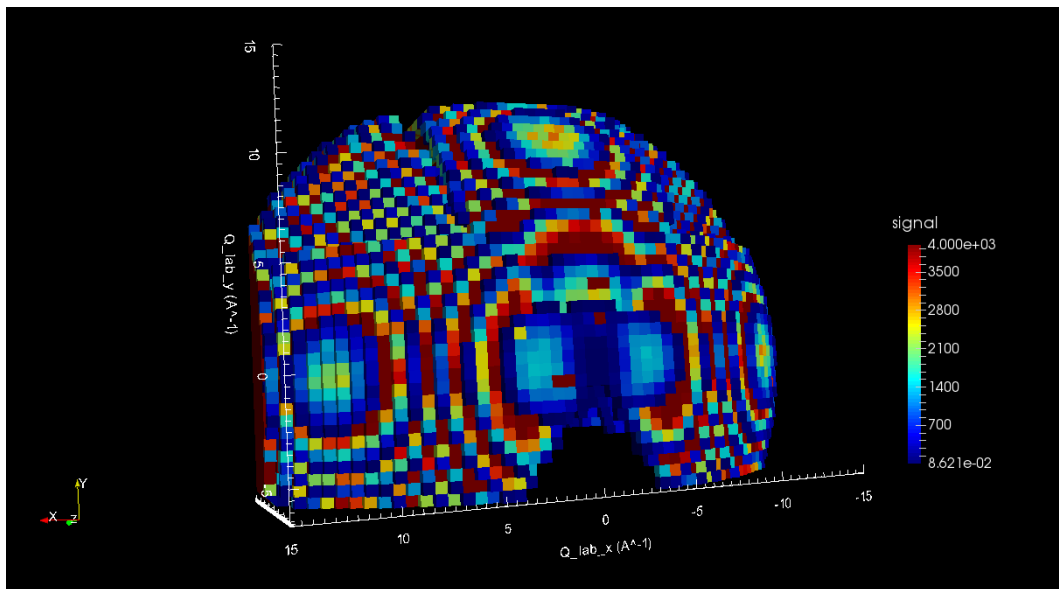
# Top Level Splitting



**Box Splitting Settings**

SplitInto	5
SplitThreshold	50
MaxRecursionDepth	13
MinRecursionDepth	1

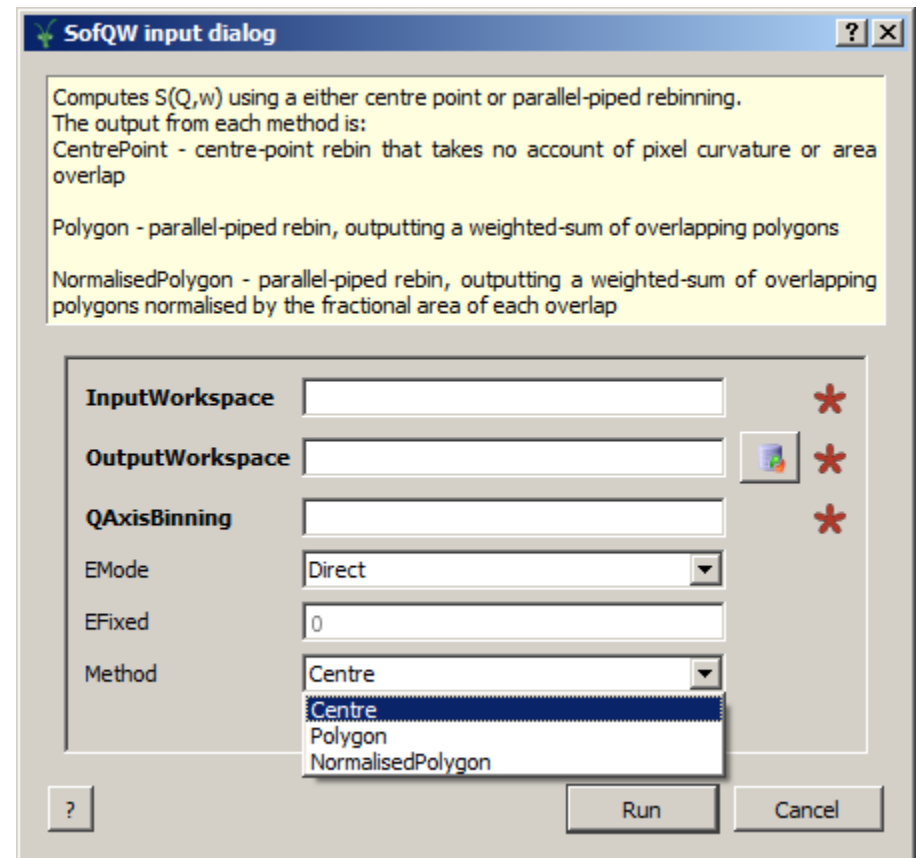
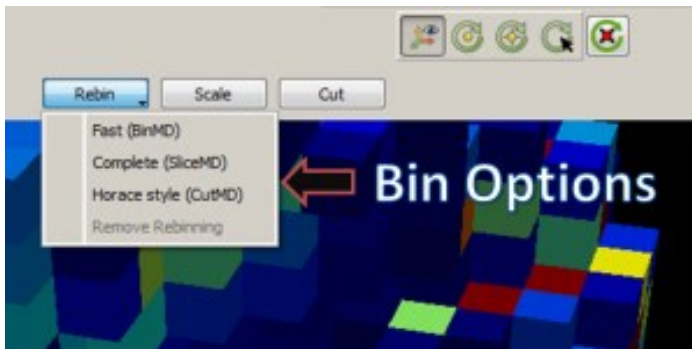
☒ TopLevelSplitting





# Other Important Changes

- **SofQW** algorithms renamed. **Method** introduced.
- Error propagation issue tracked down and fixed
- Performance improvements
- DGS planning tool
- VSI Binning Options





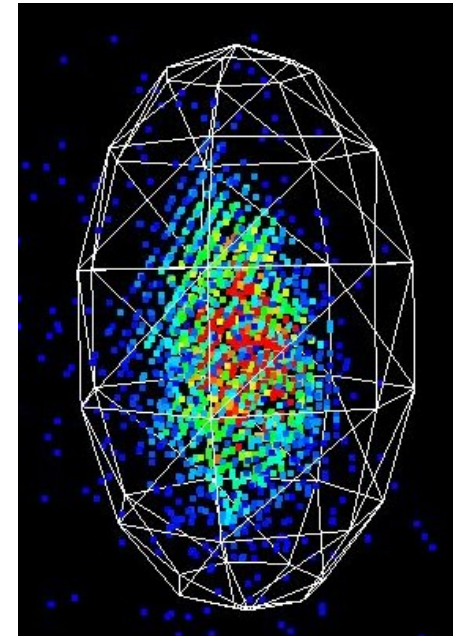
# Diffraction





# SC Peak Integration

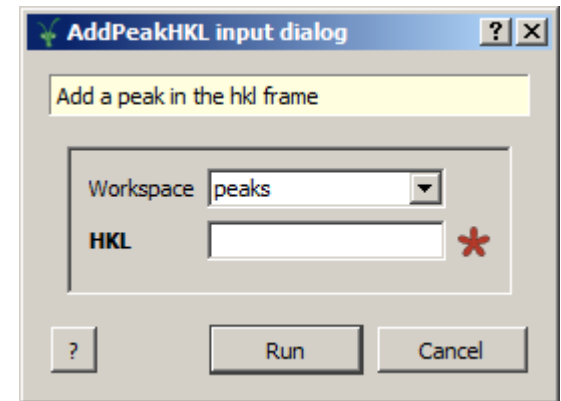
- **IntegrateEllipsoids**
  - Can now be run on 2D histogram workspaces
  - Account for weighted events
  - Now parallel processes as part of the PCA
- **IntegratePeaksMD**
  - Fix to the adaptive Q radius calculation
  - Caches used for speed improvement
- **PeakShape** introduced
  - Frame
  - Algorithm + Version
  - Flexible + extendable shape definition
  - Used in the 3D visualisation tools





# New Algorithms

- **StatisticsOfAPeaksWorkspace**
- **AddPeakHKL**
- Horace style algorithms
  - **CutMD,**
  - **CreateMD,**
  - **SmoothMD,**
  - **IntegrateMDHistoWorkspace**





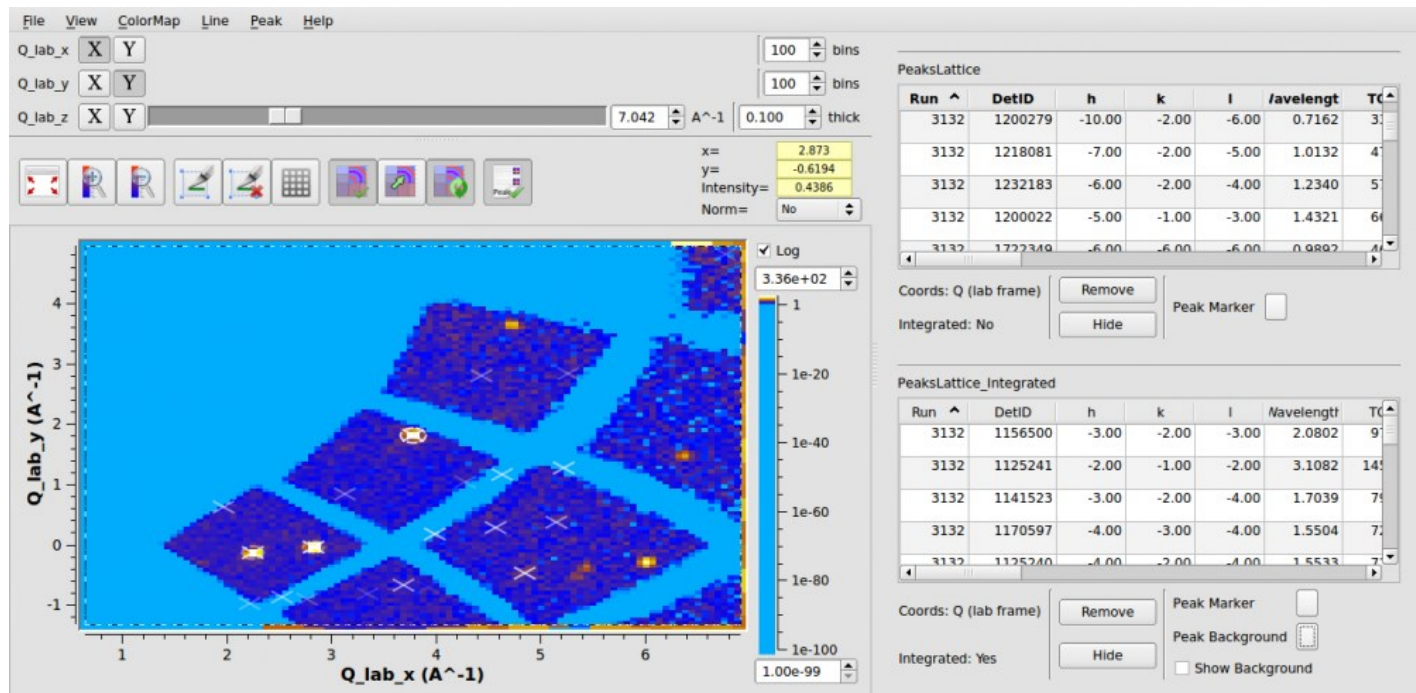
# PeaksViewer for VSI

- Demo



# PeaksViewer

- PeaksViewer mode of SliceViewer now supports drag-drop
- PeaksViewer is now completely synchronised via MantidPlot's PeaksWorkspaces
- Up-down keyboard keys on the mini-table give zoom-to-peak feature





# Next Release



# Release v3.5

- Planned Release Date: Monday 5<sup>th</sup> October 2015
- Mantid Roadmap
  - <http://trac.mantidproject.org/mantid/roadmap>



Thank you

