MANTID

Mantid Release Presentation

Release 3.4
ISIS

ISIS

ESS EUROPEAN SPALLATION SOURCE

Tessella
Technology & Consulting

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

What is this meeting

- Release 3.4
  - Released on Monday 18th 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
  - More details at www.mantidproject.org

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User Interface

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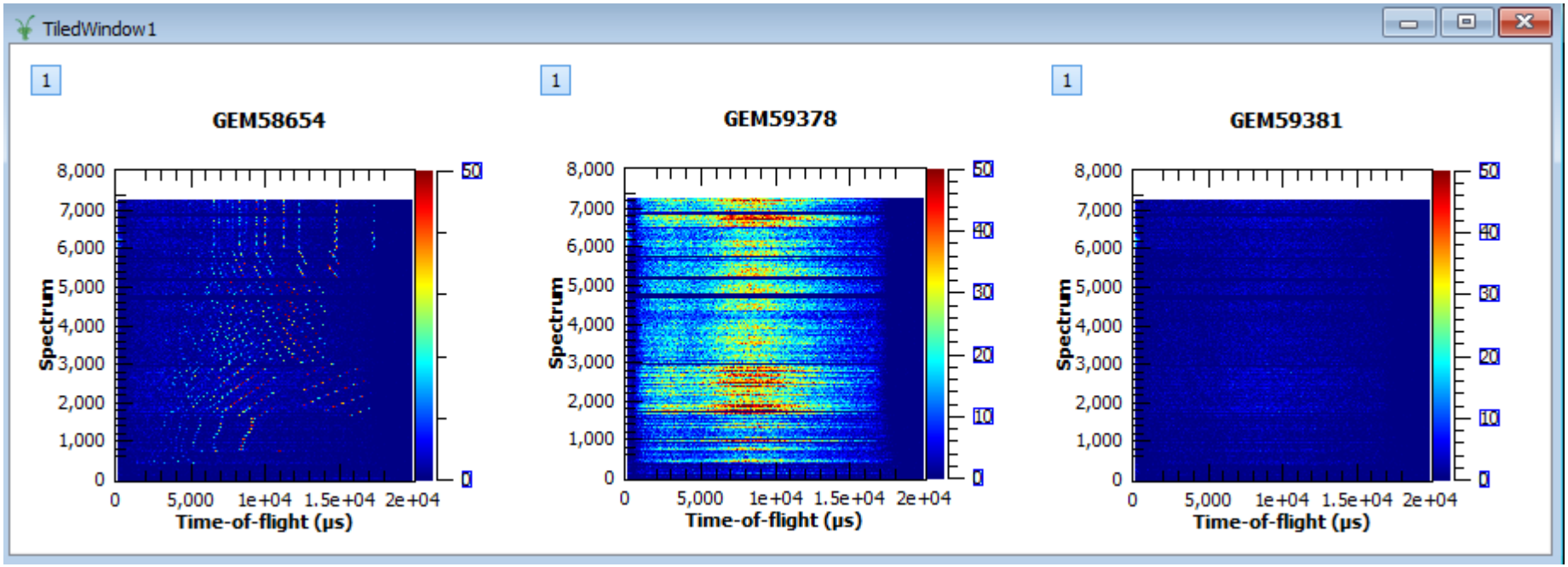
Tiled Windows



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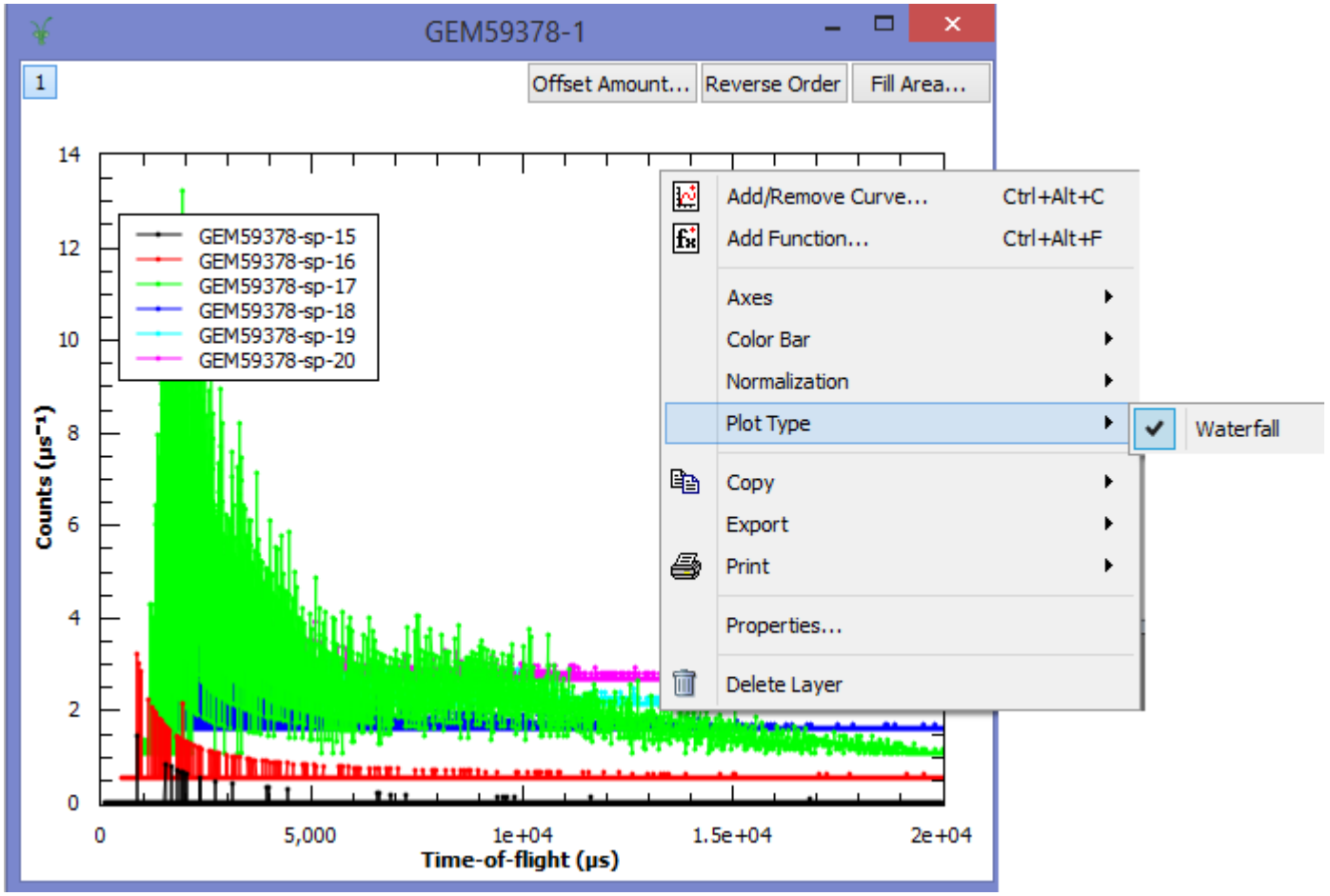
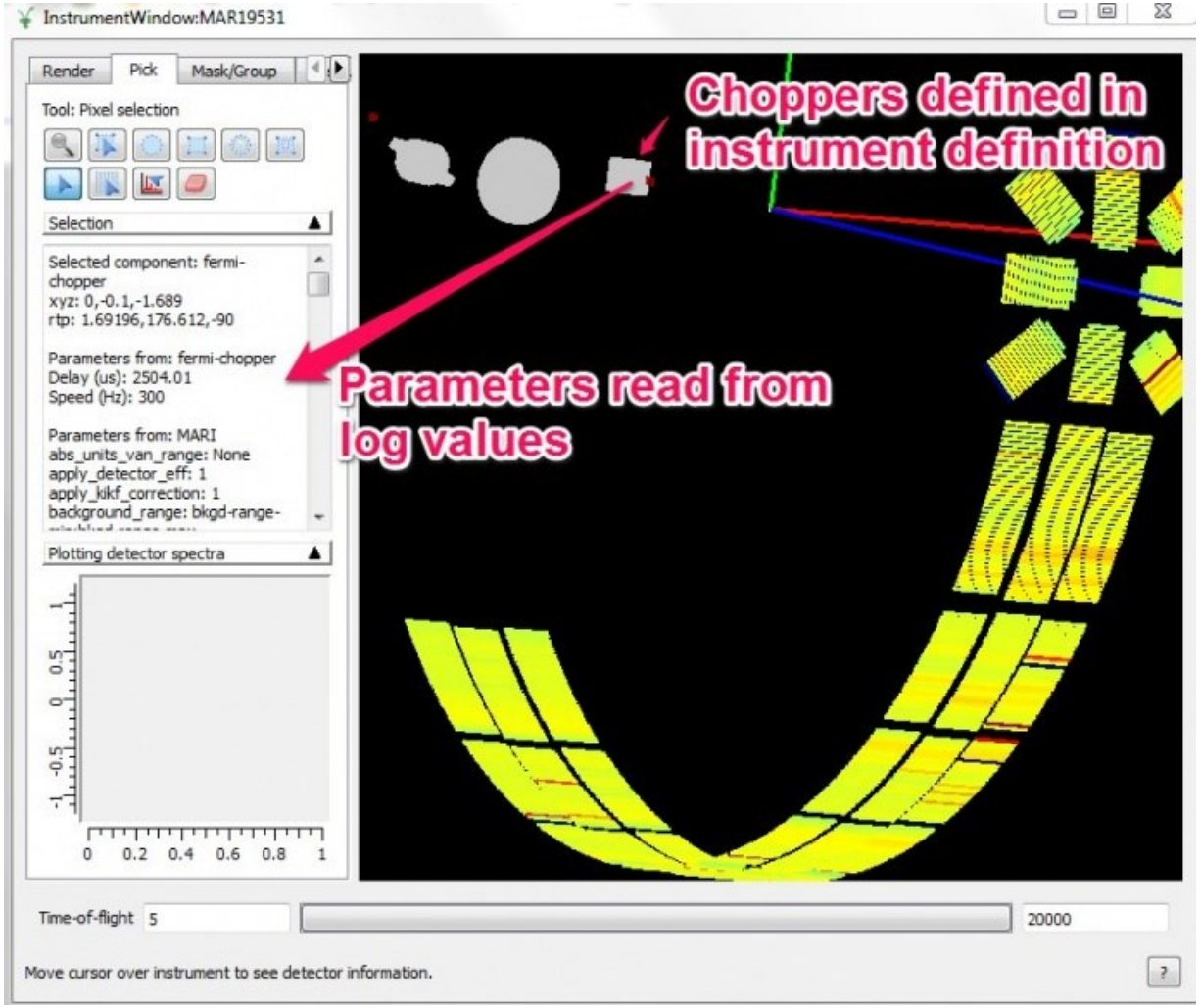
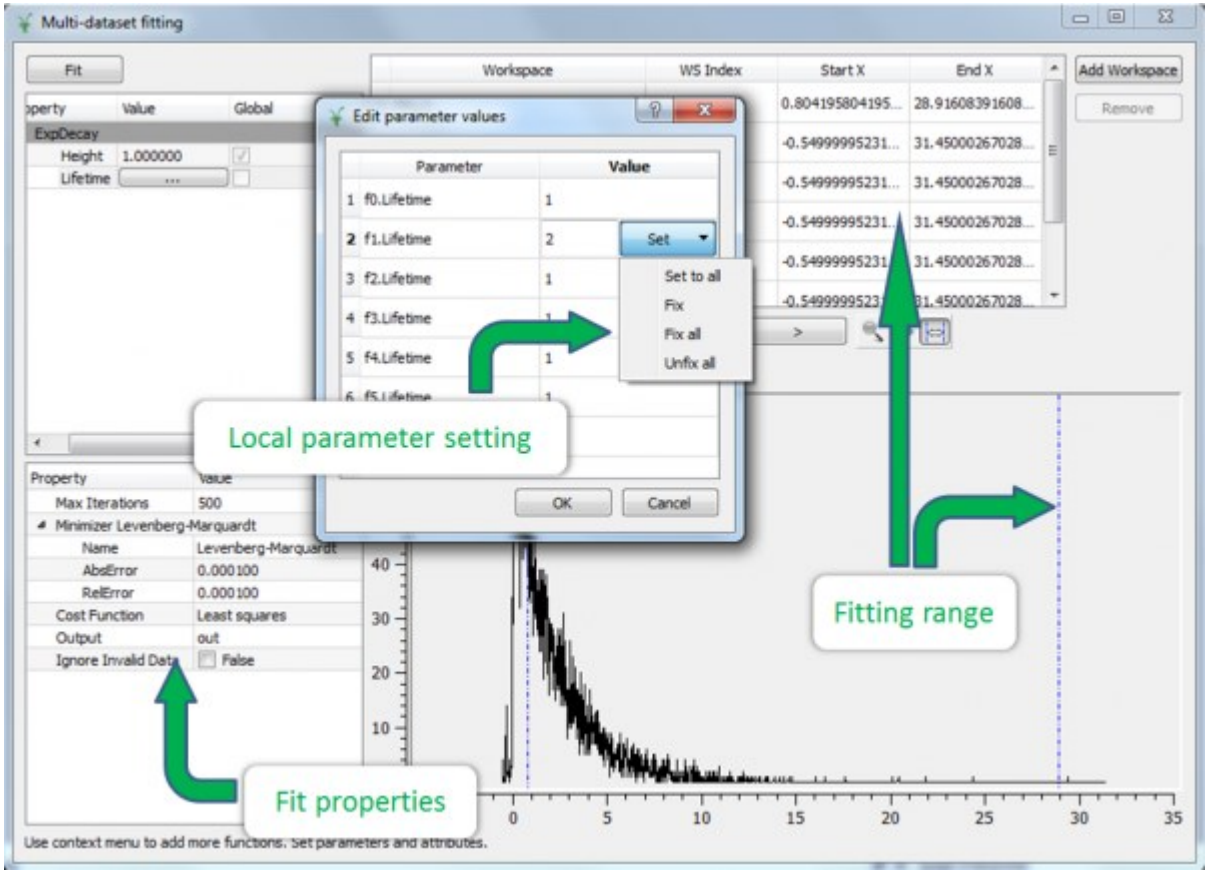
Water Fall Plots



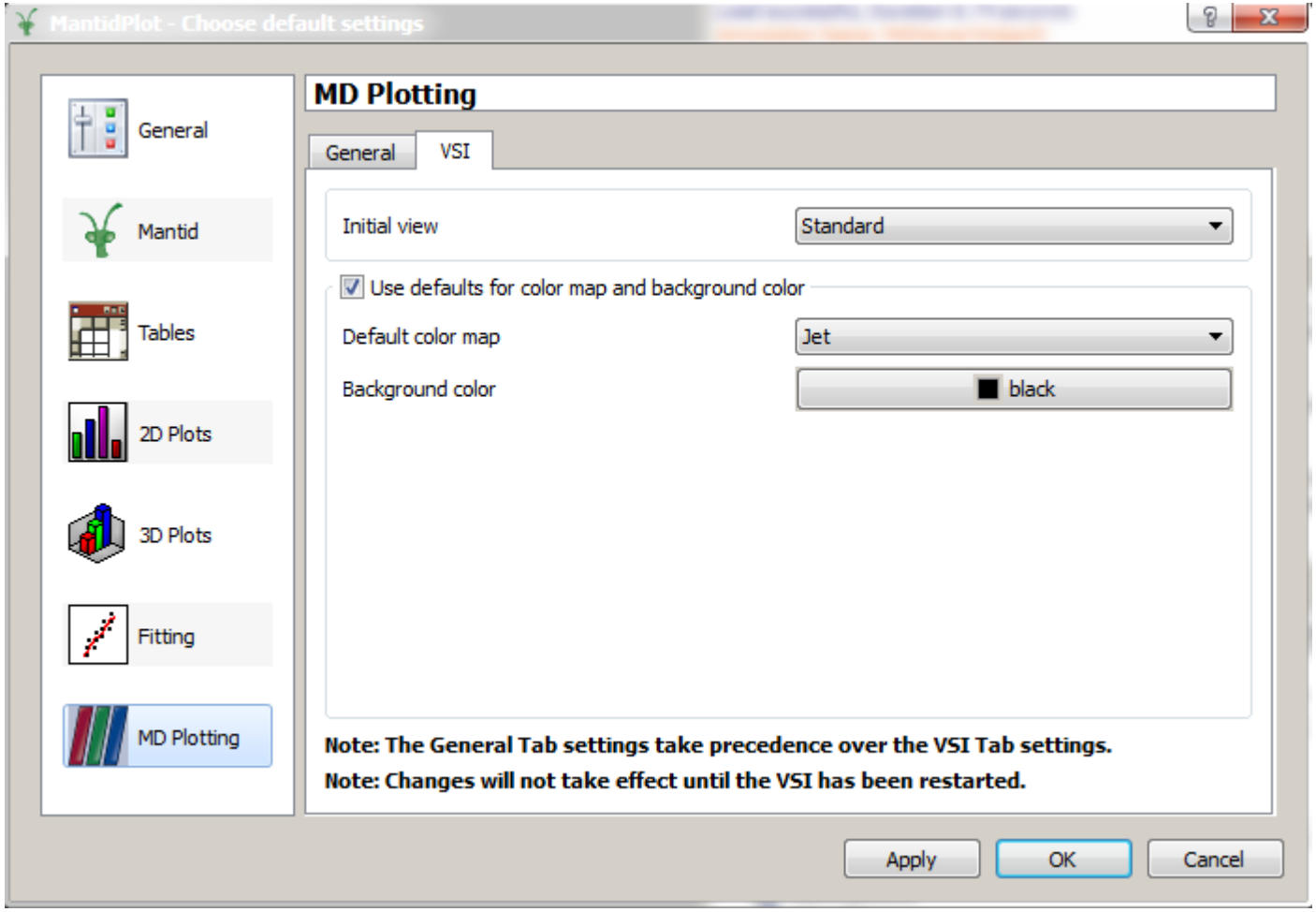
Non-detector Components



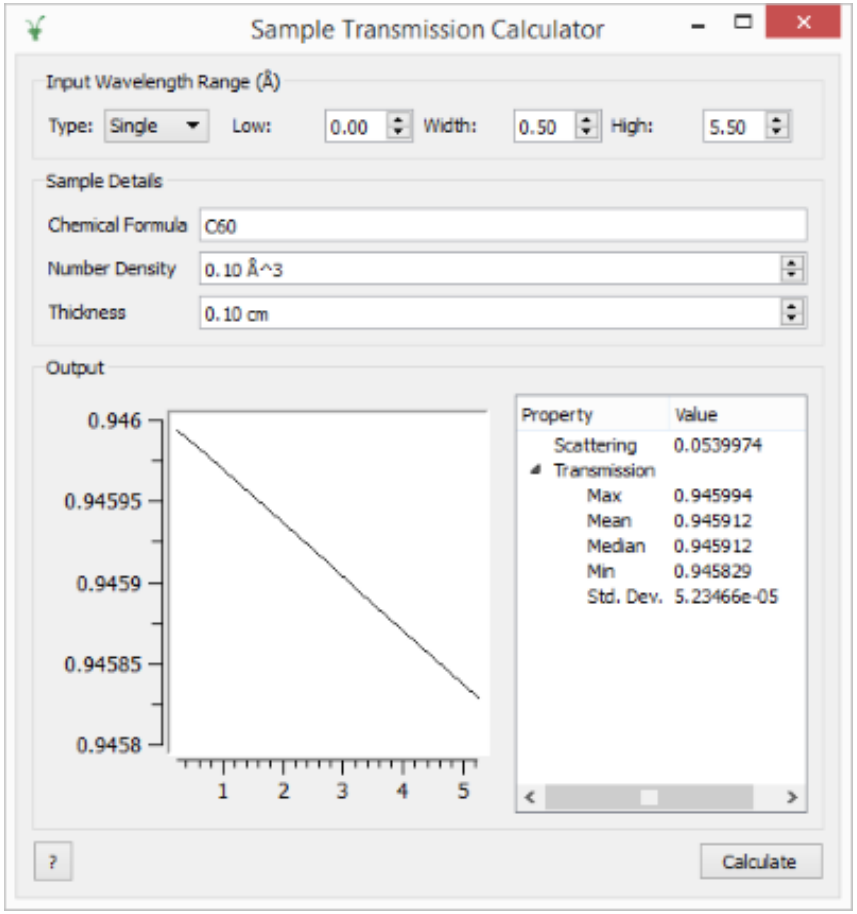
Multi-data Fitting



MD Viewer (VSI)



New Sample Transmission Calculator



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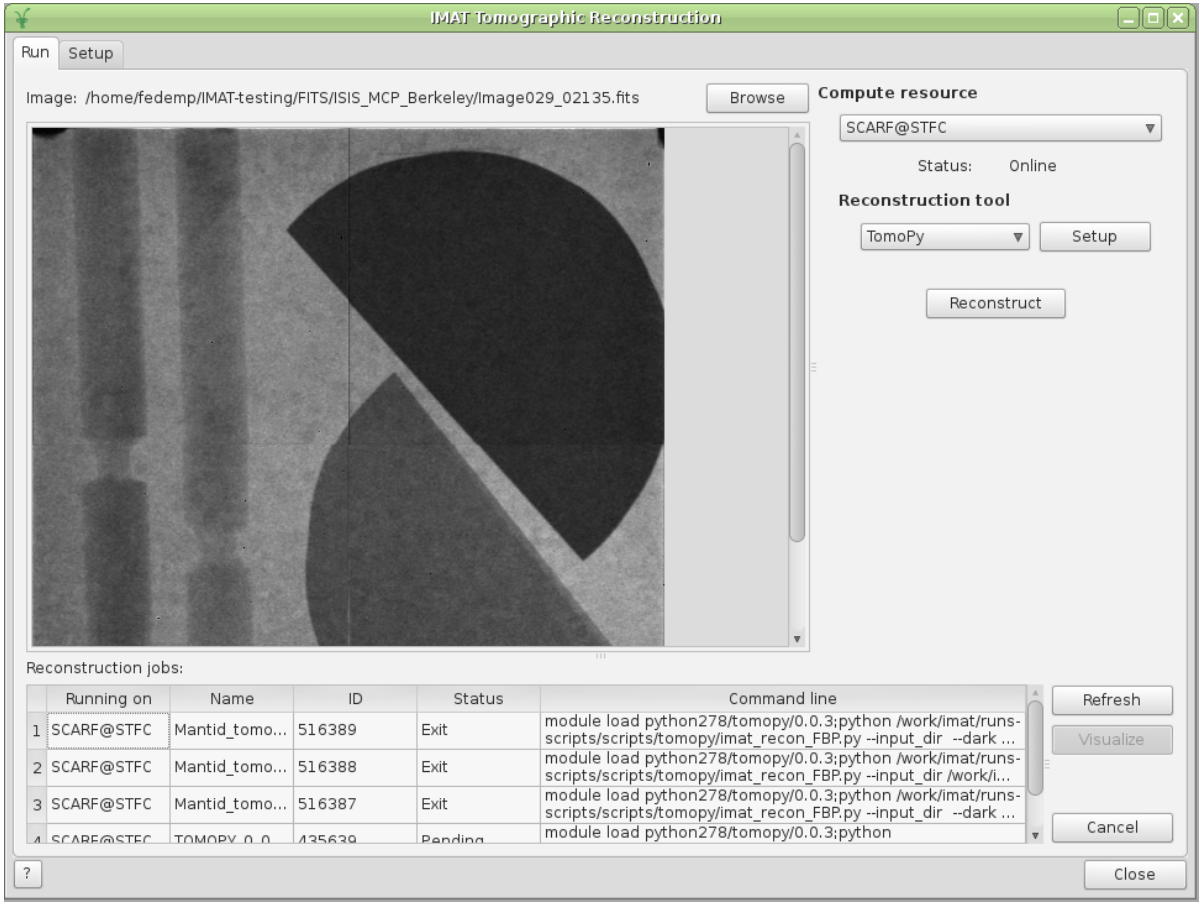
Other Important Changes

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



Framework

Framework – Improvements

- ParaView bundled with the installation packages

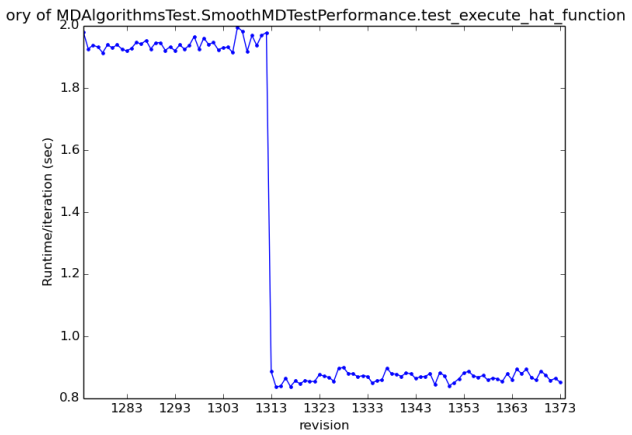
- Instrument definitions
  - LET, ALF and others at SNS updated
  - You get these updates automatically since v3.3
- Infrastructure for distributed computing

SCARF
Scientific Computing Application Resource for Facilities

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

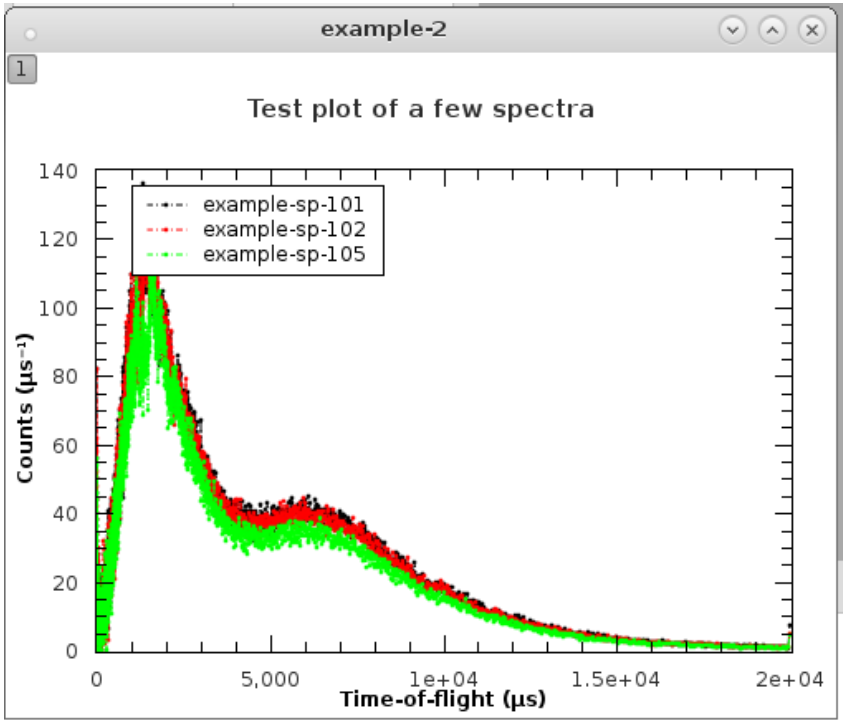
Performance Improvements

- 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**)




```
In [26]: example = Load("MAR11060.raw", OutputWorkspace="example")
In [27]: lines = plot(example, [100, 101, 104], linestyle='-.')
In [28]: title('Test plot of a few spectra')
```

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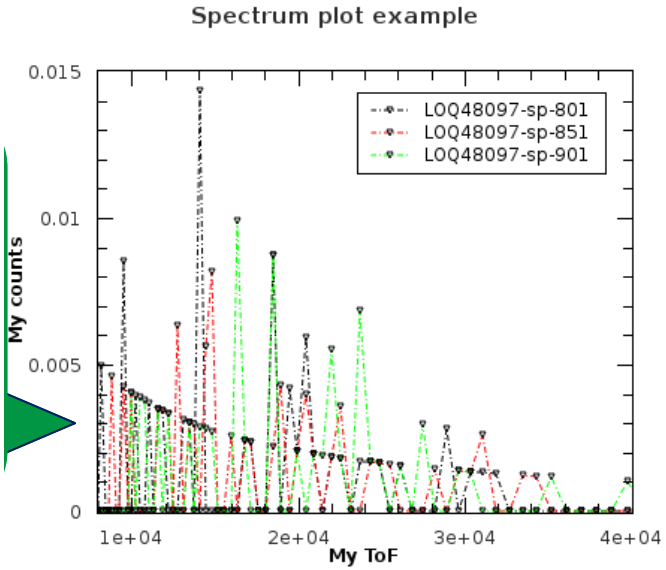
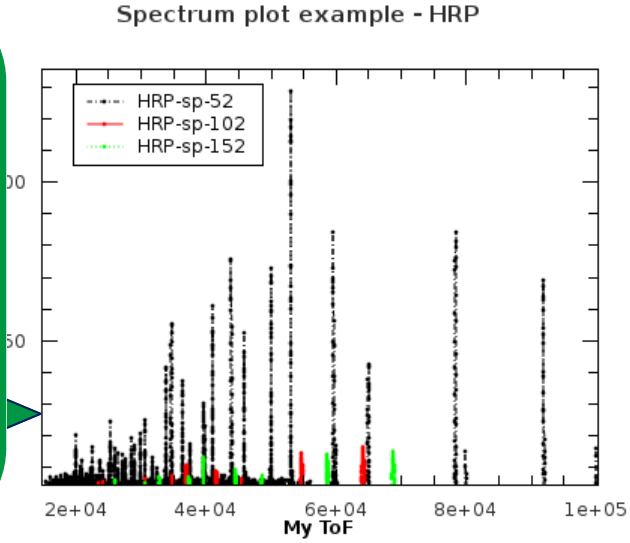
Python Plotting Command Line Interface

- 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)
```

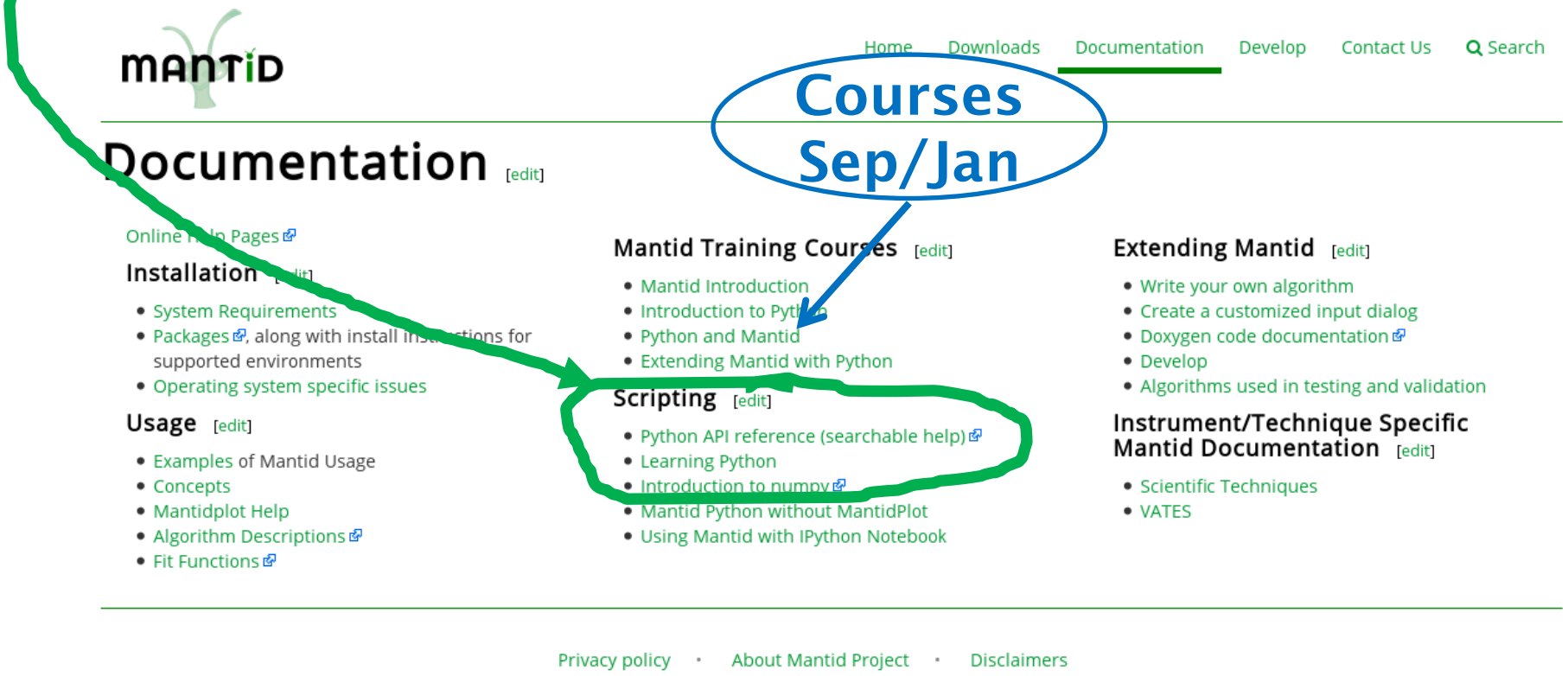


- Object-oriented interface (Figure, Axis, Line2D, etc.):



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



Indirect Inelastic

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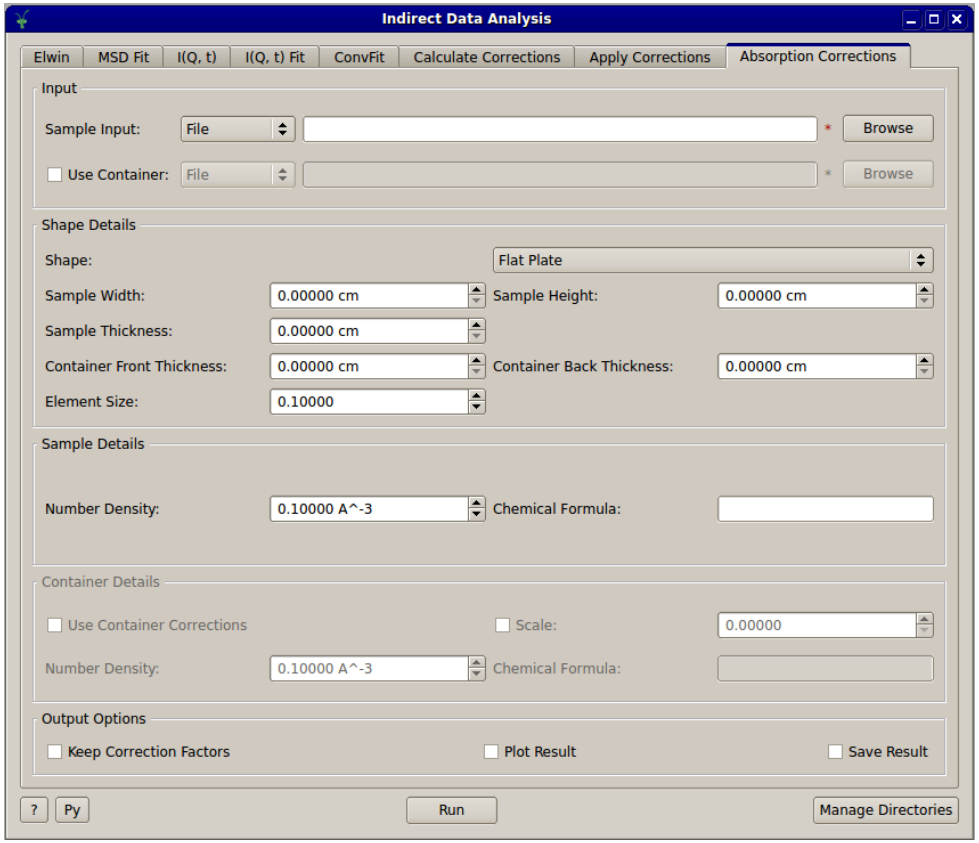
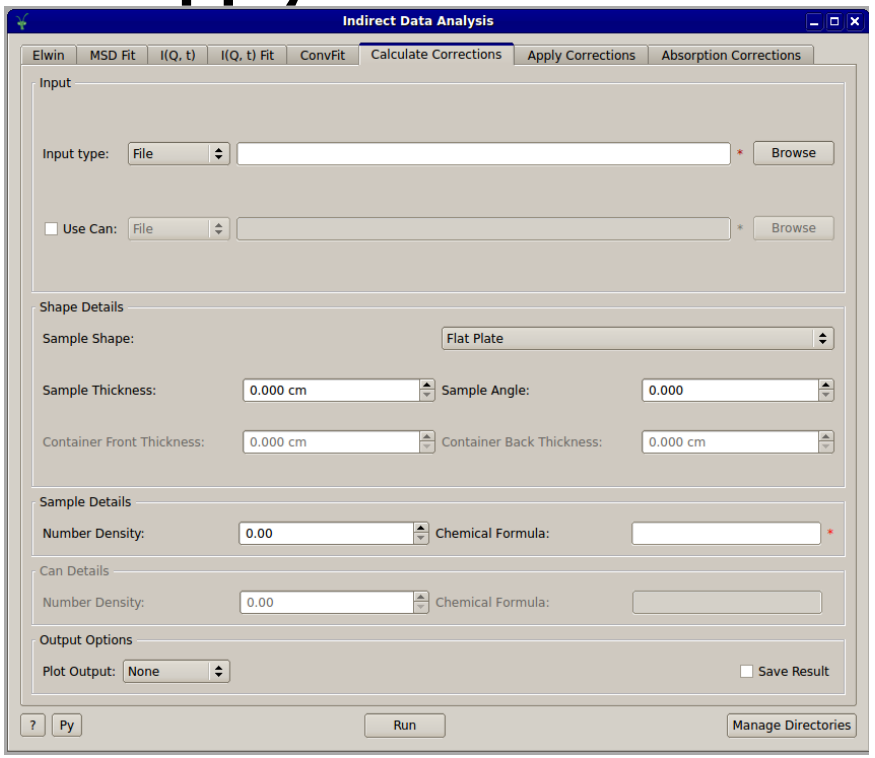
Absorption Corrections

- 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



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



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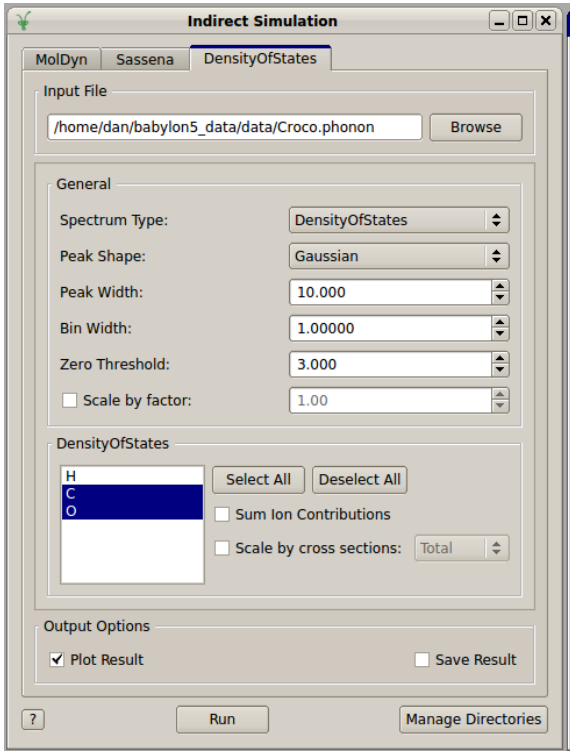
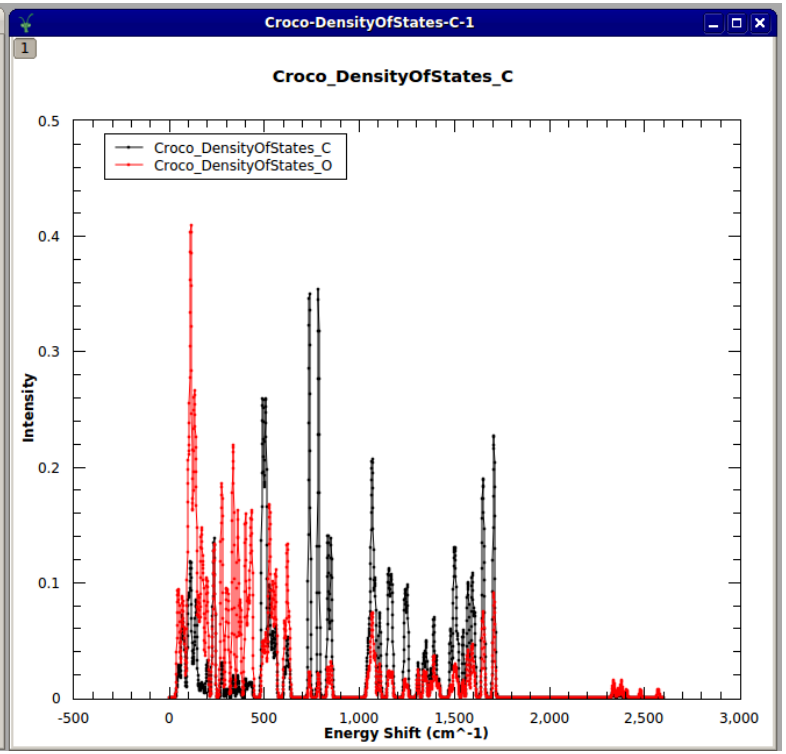
Interface Updates

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





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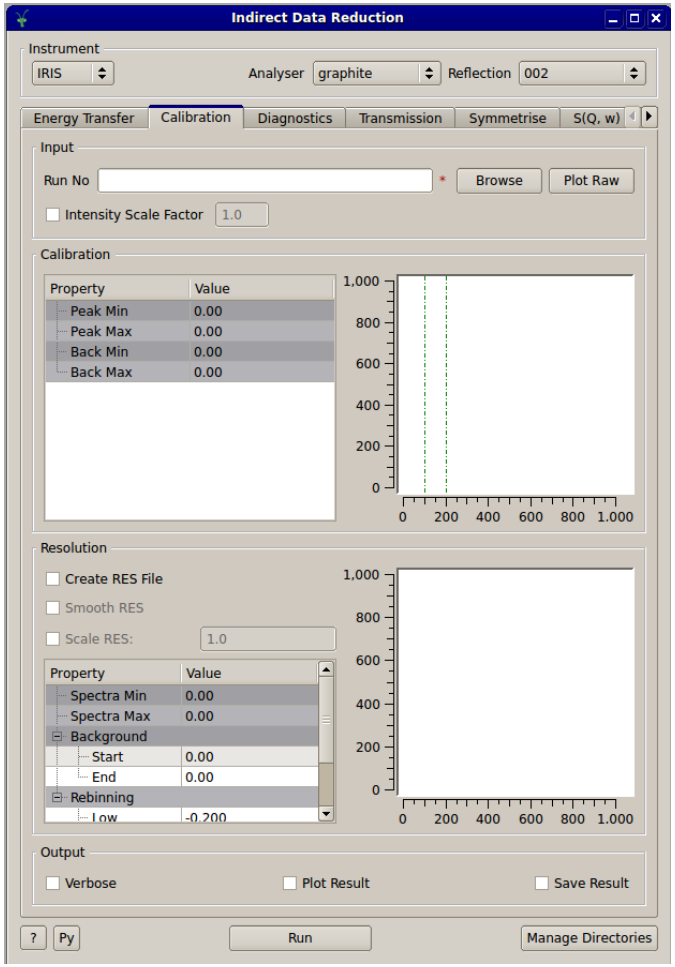
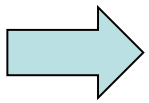
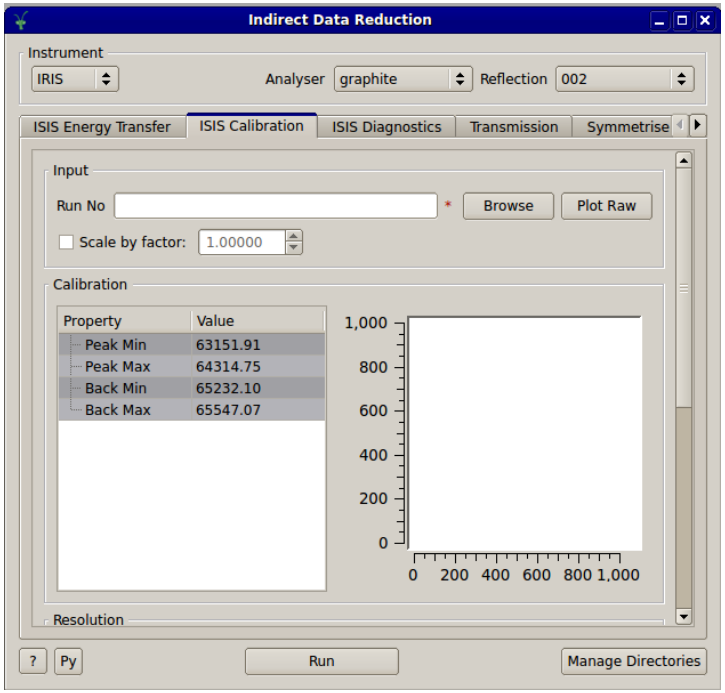
Interface Updates

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

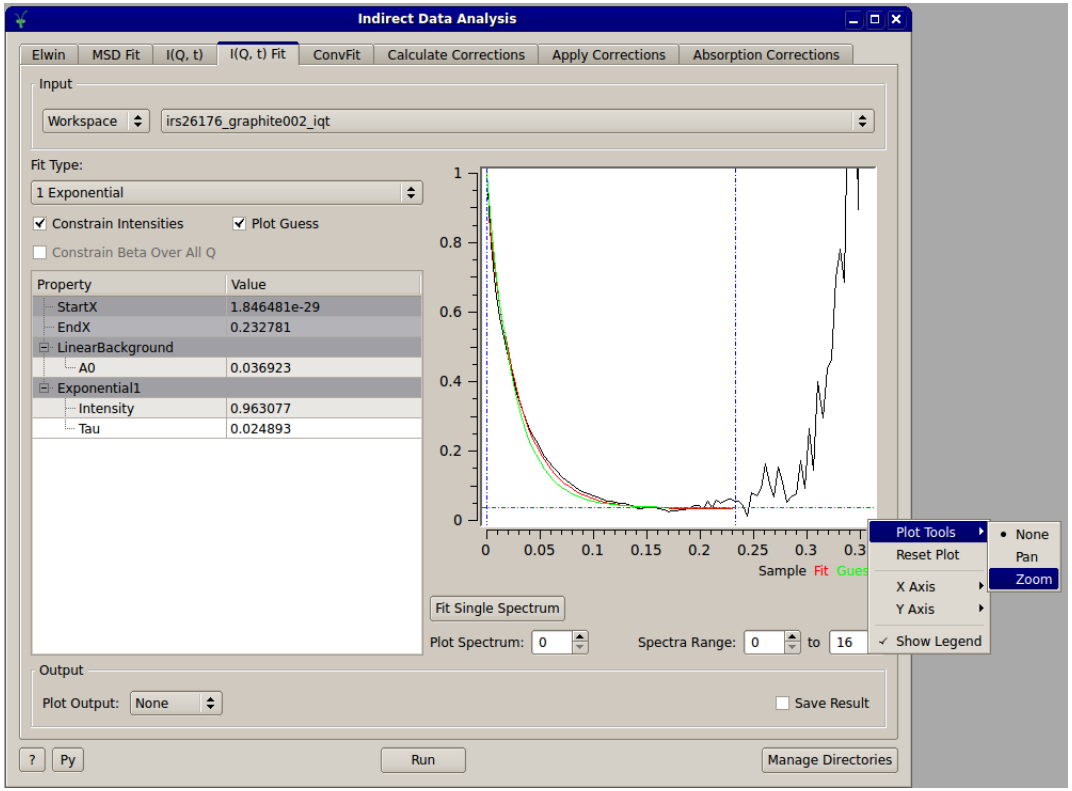






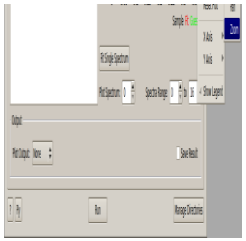
Interface Updates

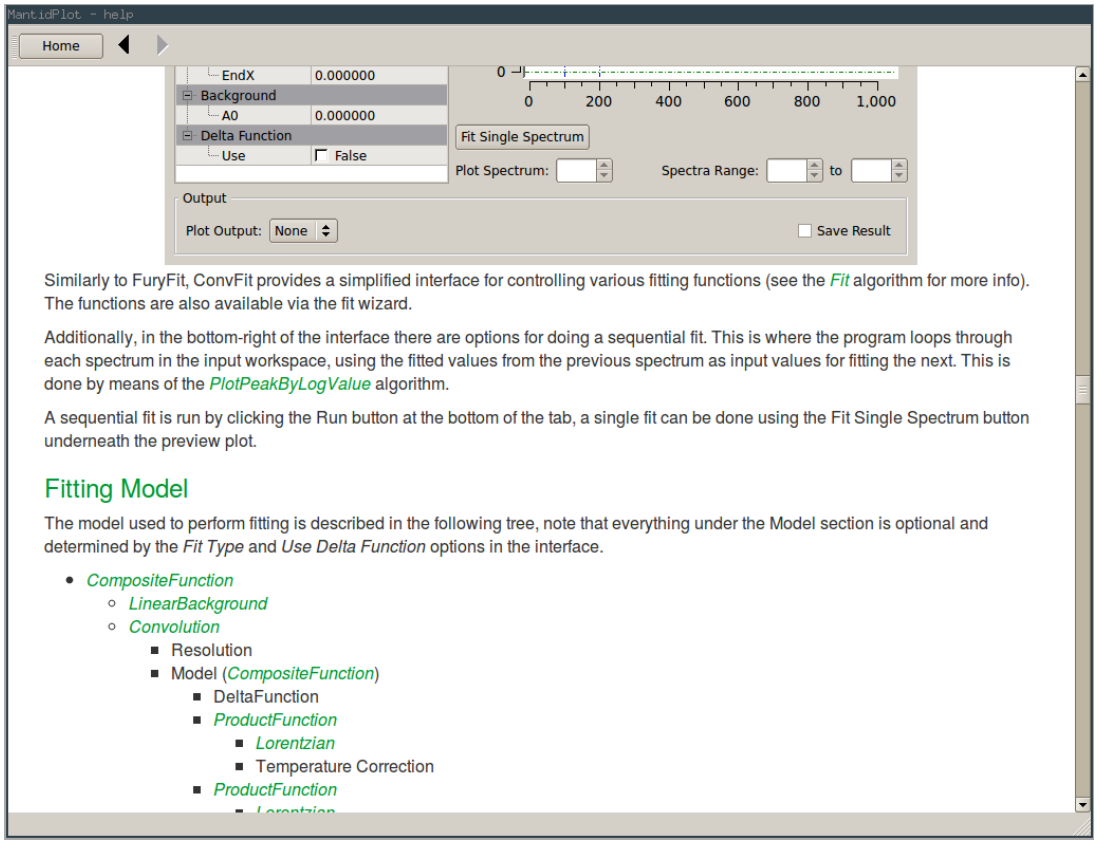
- Standard preview plot widget in all indirect interfaces
- Supports:
  - Changing axis scales
  - Pan tool
  - Zoom tool
  - Automatic zooming
  - Legend toggle



Interface Documentation

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





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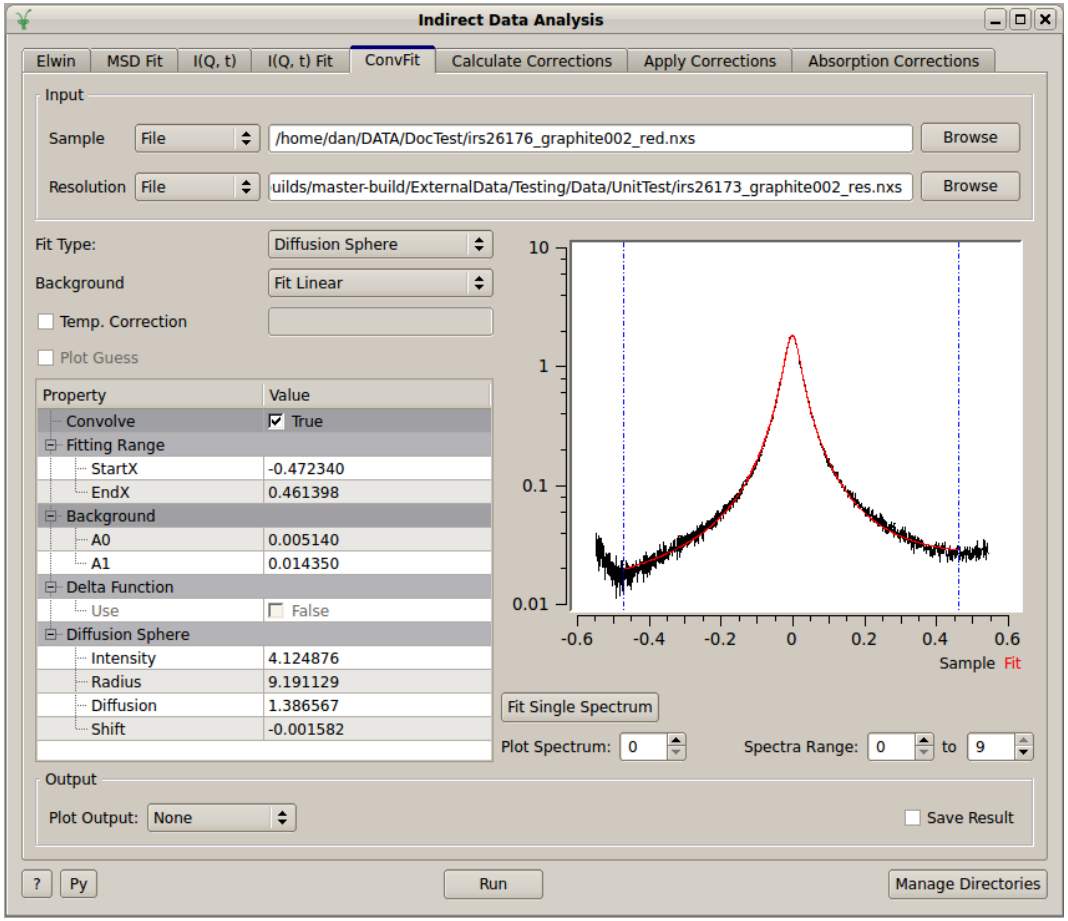
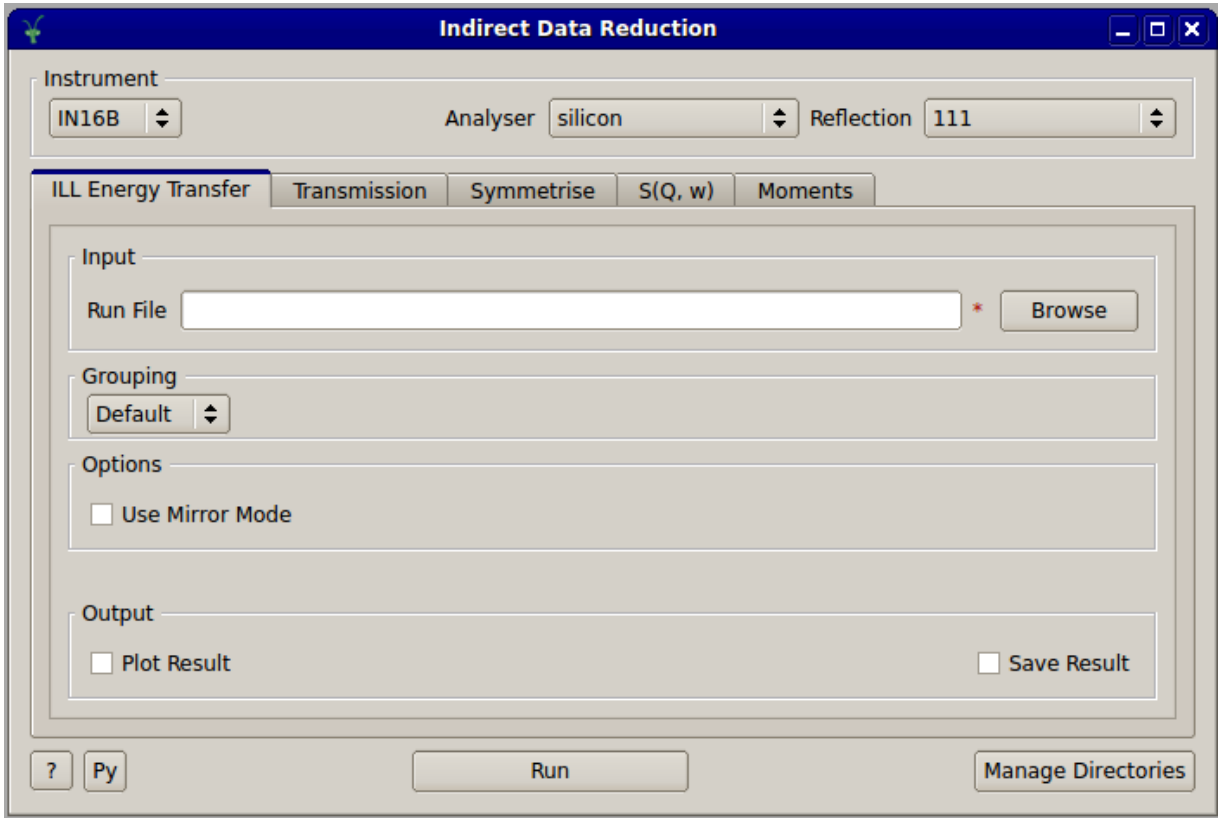
ConvFit

- 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

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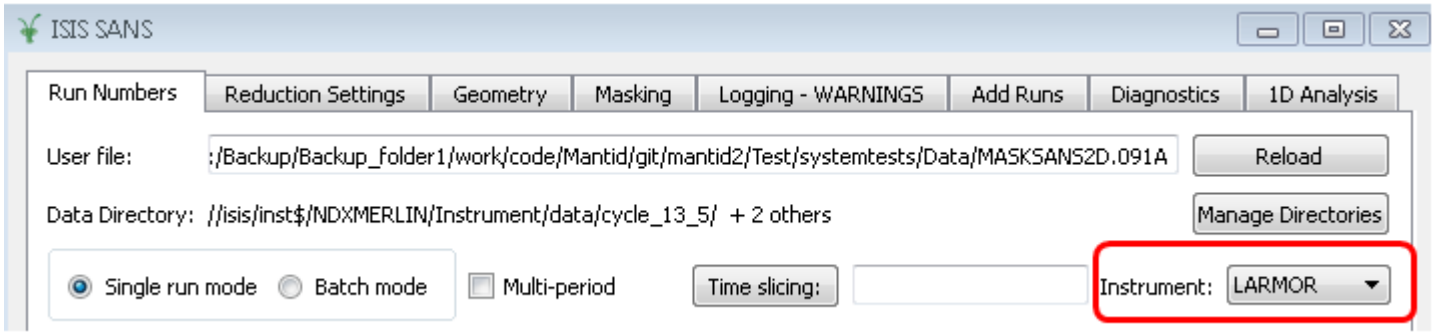
SANS

ISIS SANS GUI

- **Support for LARMOR**



- **Allow added event files to be reduced !**

SasView

- **Overhaul of documentation**
- **New models added**

Muon

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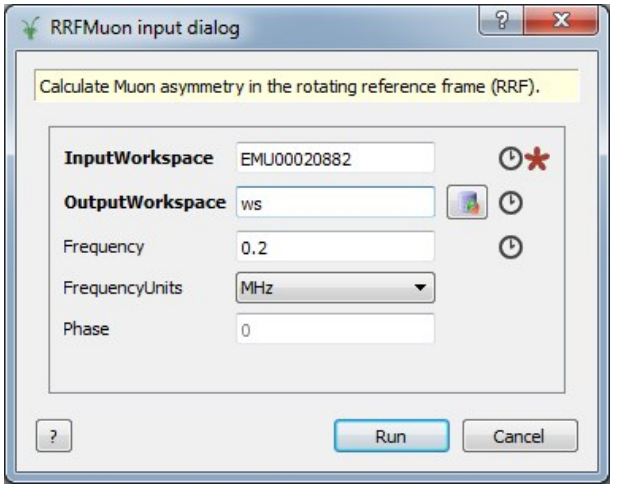
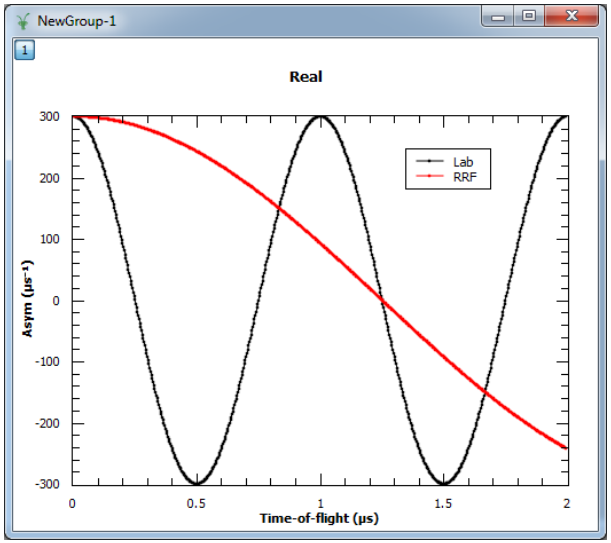
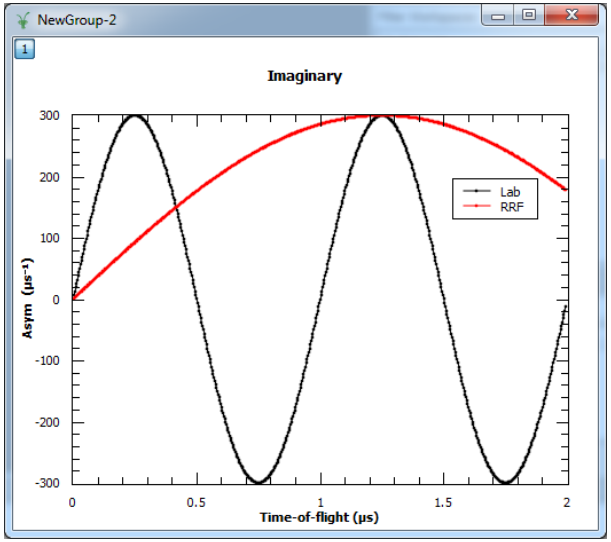
New RRFMuon algorithm

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







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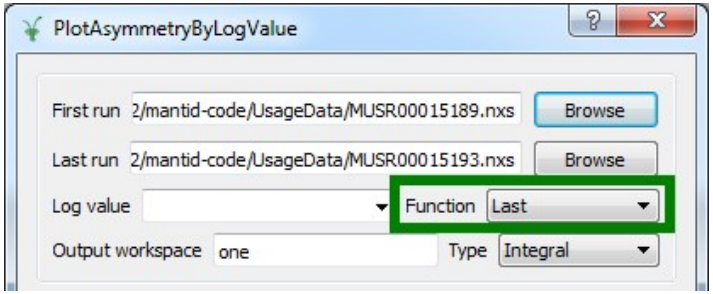
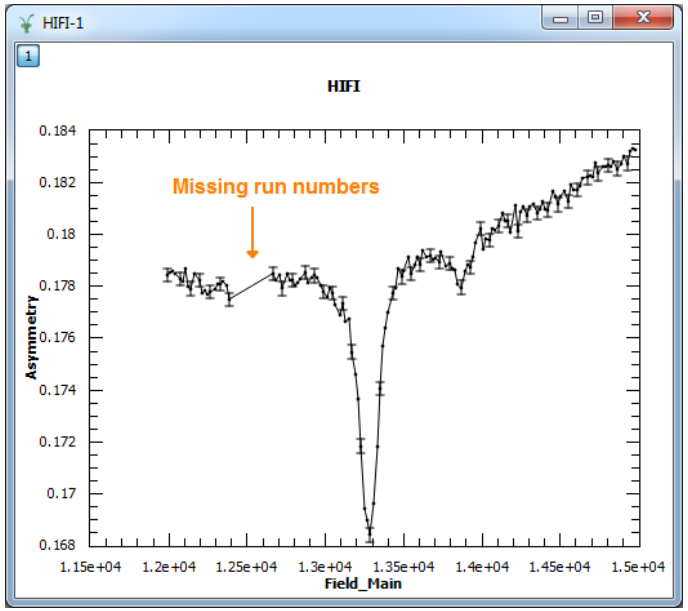
Existing algorithms

- 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

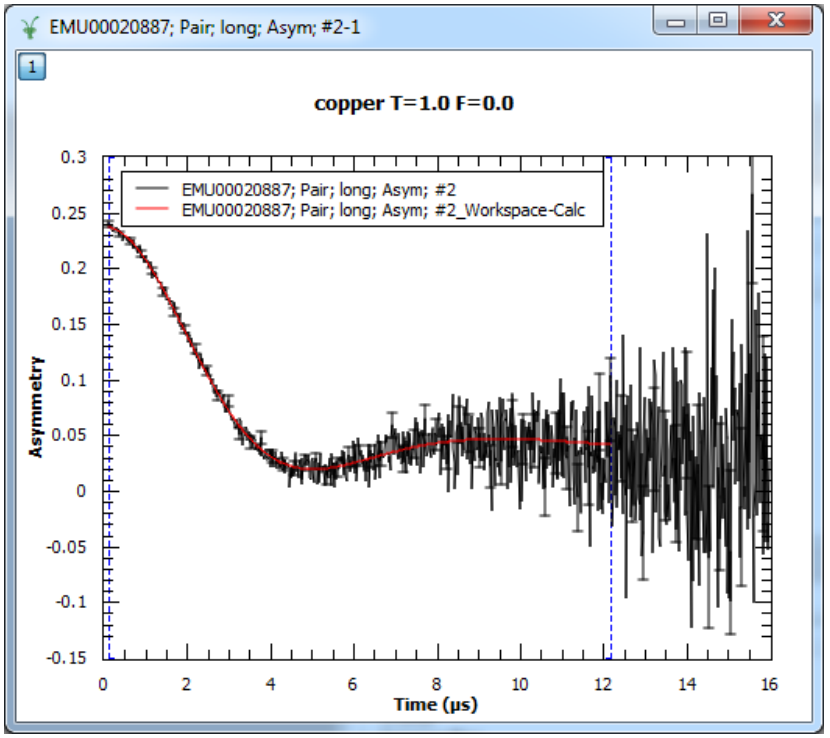




DynamicKuboToyabe fitting function

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

- Muon category
- Fitting parameters:
  - Asymmetry A
  - Local field Δ
  - External field F
  - Hopping rate ν
- Attribute:
  - Bin width



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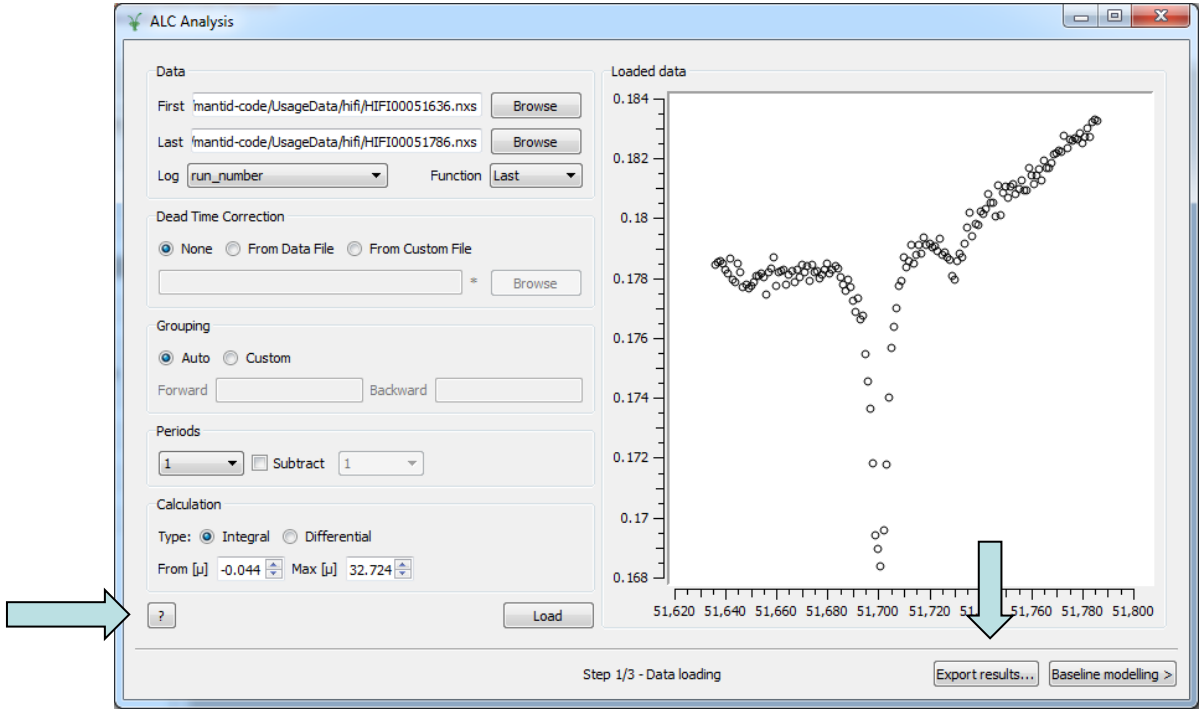
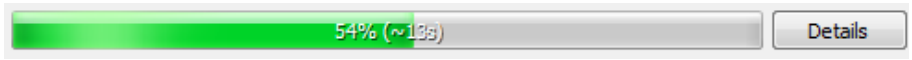
ALC Interface

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



- DataLoading:
  - Progress bar
  - Missing options added



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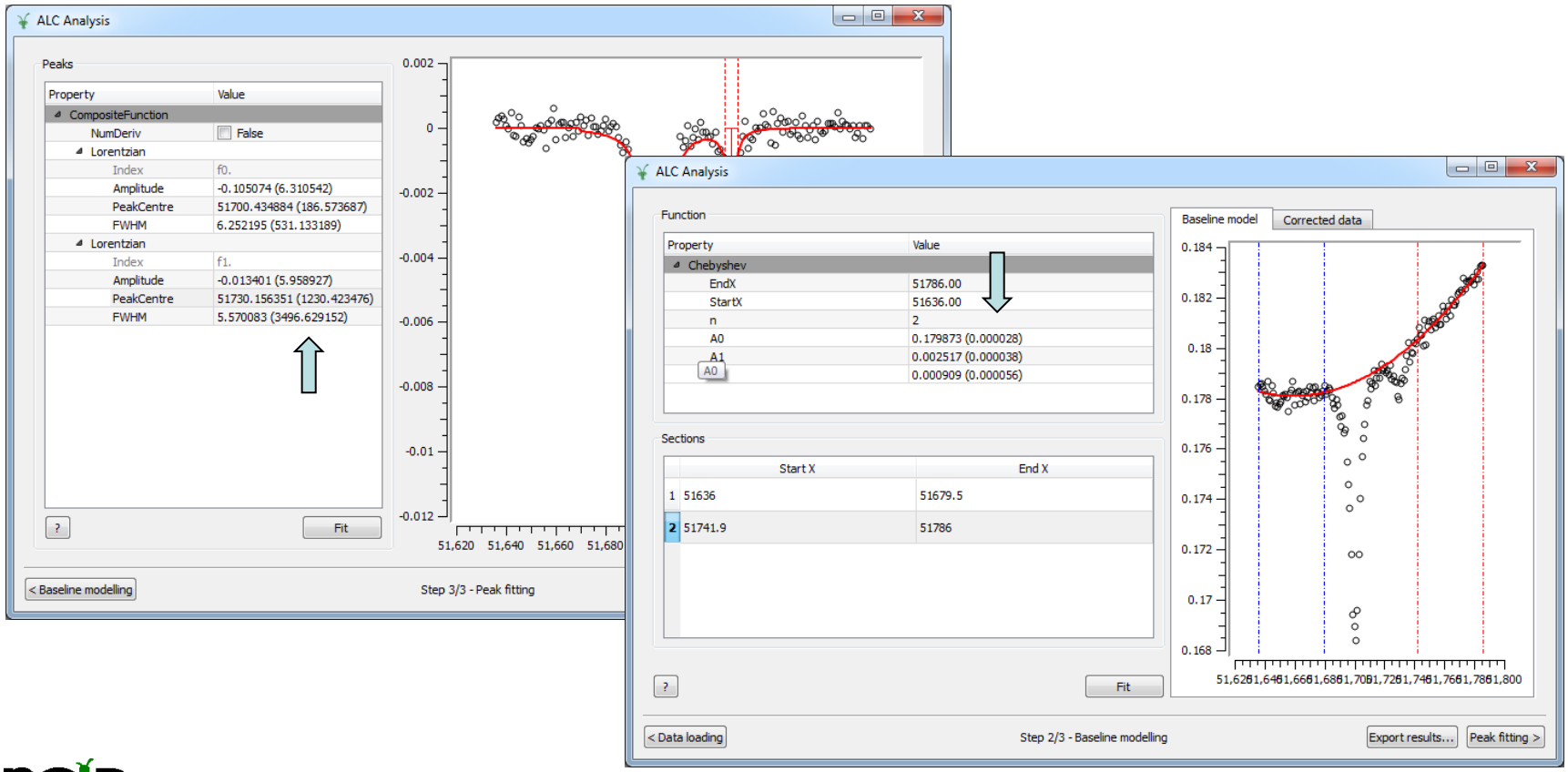
ALC Interface

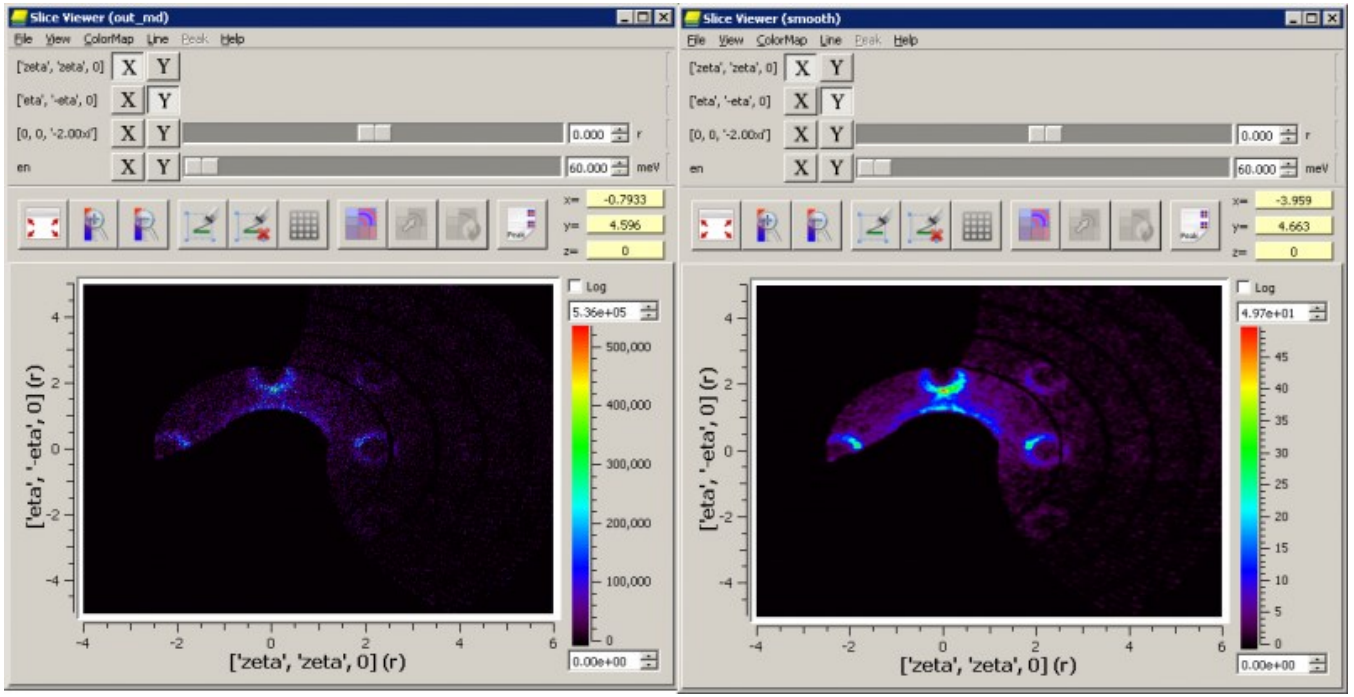
- Parameter errors
- BaselineModelling: range selectors



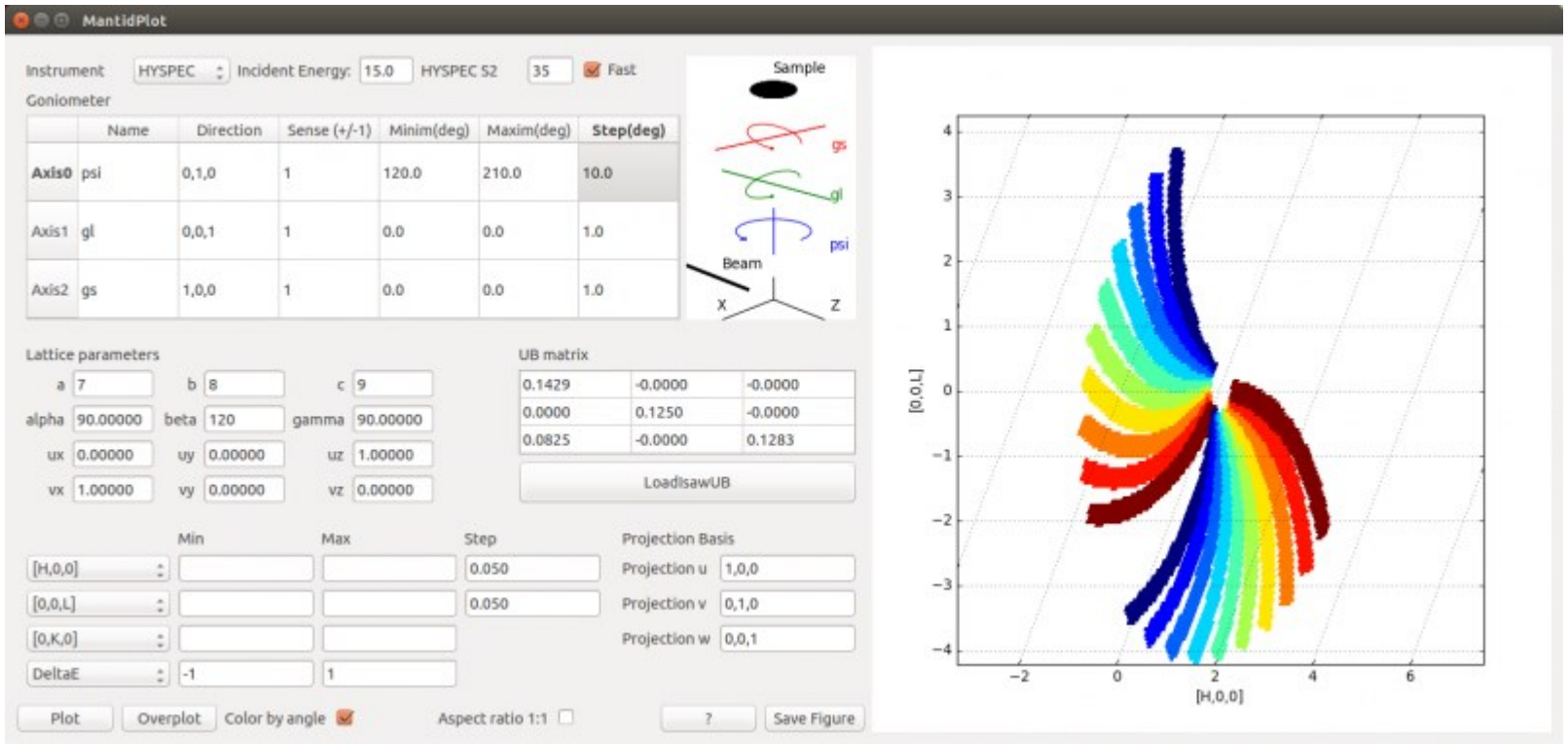
Direct Inelastic

Horace Style Commands

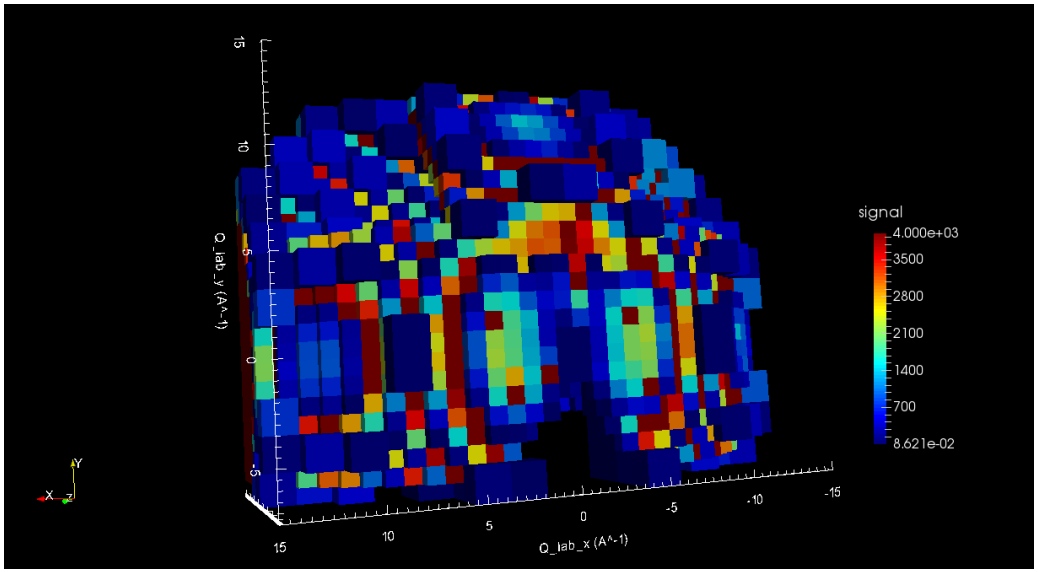
- **CutMD** equivalent to **cut_sqw**
  - Introduction of Horace style Projections into Mantid
- **CreateMD** equivalent to **gen_sqw**
  - Creates merged workspaces in one step
  - With a file-backed mode
- **SmoothMD** equivalent to **smooth**
- **IntegrateMDHistoWorkspace**

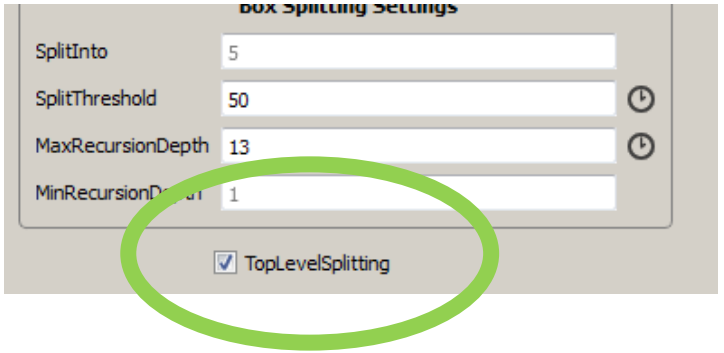


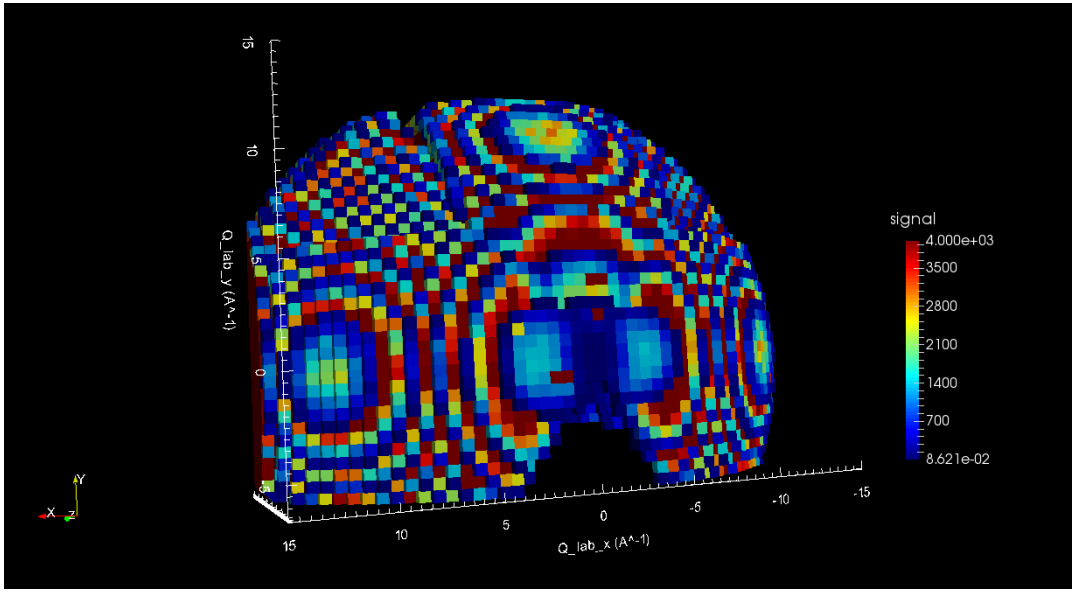
New DGS Planner



Top Level Splitting







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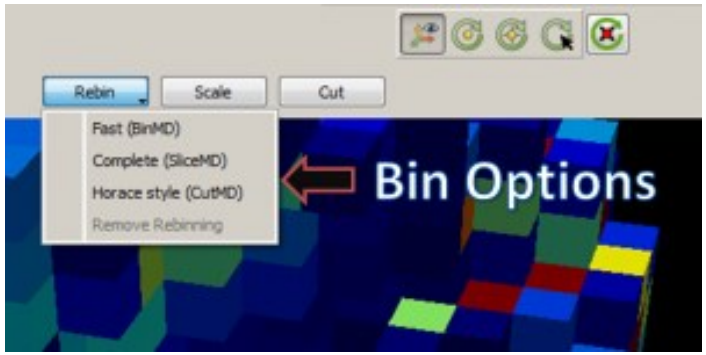
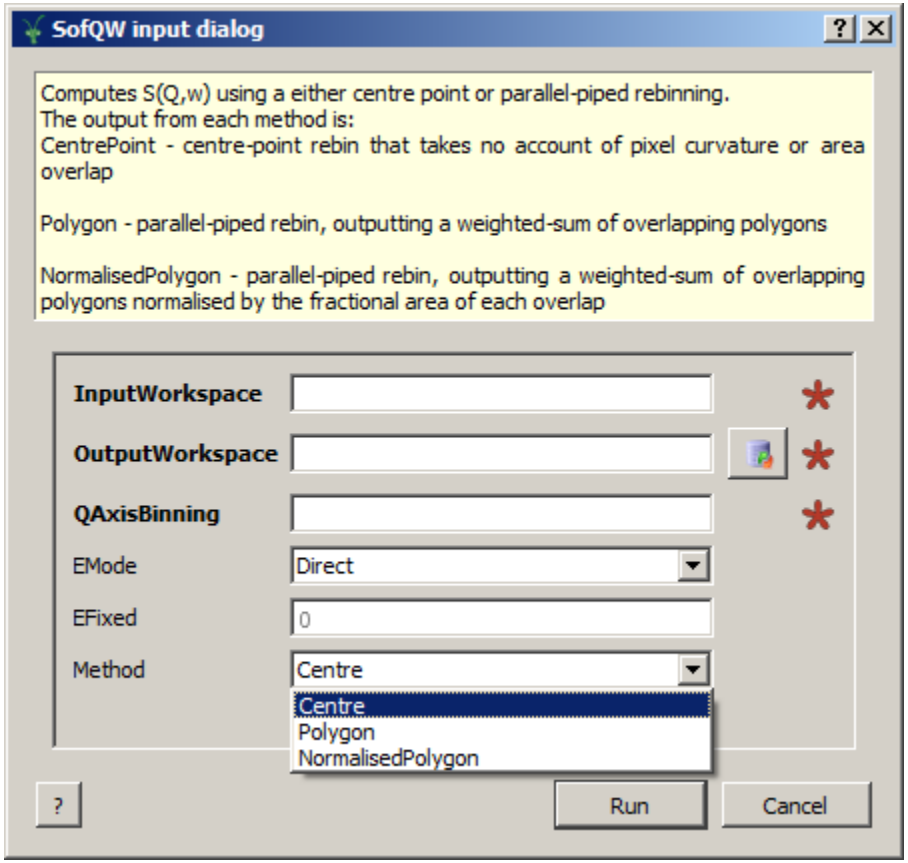
Other Important Changes

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

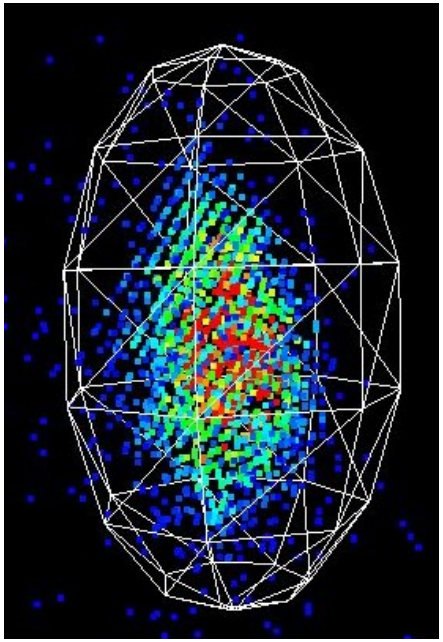




Diffraction

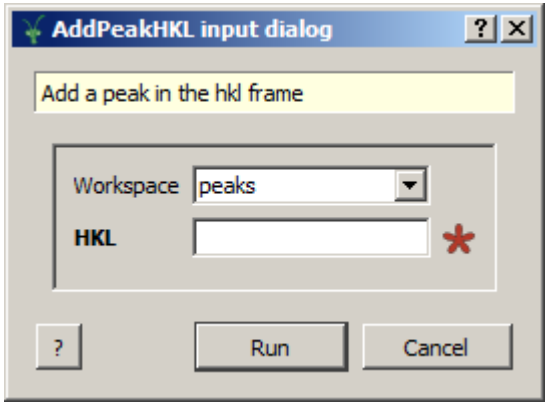
SC Peak Integration

- **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**



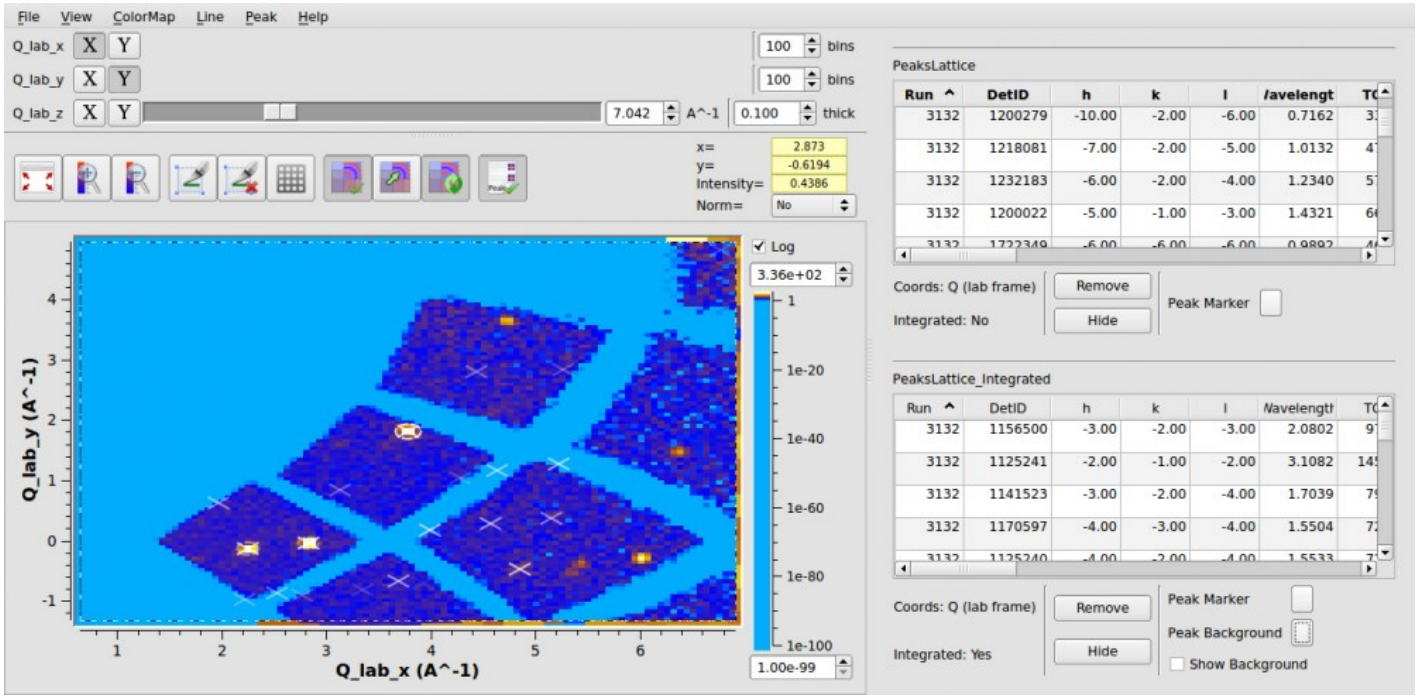
PeaksViewer for VSI

- Demo

MANTID

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 5th October 2015
- Mantid Roadmap
  - http://trac.mantidproject.org/mantid/roadmap

Thank you