

Mantid Release Presentation

Release 3.5
ISIS



What is this meeting

- Release 3.5
 - Released on Monday 5^h October
 - Present the changes and improvements



Training Courses

- Dates
 - Last Course
 - September 2015
 - Next courses
 - Jan/Feb 2016



- To Book
 - Email: nick.draper@stfc.ac.uk
 - More details at www.mantidproject.org



Supported Platforms

- Staying the same
 - RHEL 6 64bit
 - RHEL 7 64bit
 - OSX Mountain Lion +
 - Windows 7 64 bit
 - Ubuntu 14.04 64 bit



RED HAT
ENTERPRISE
LINUX 7



OS X Mountain Lion



- Limited support for
 - Windows 8 64 bit
 - Fedora 20



Windows 8

fedora 20

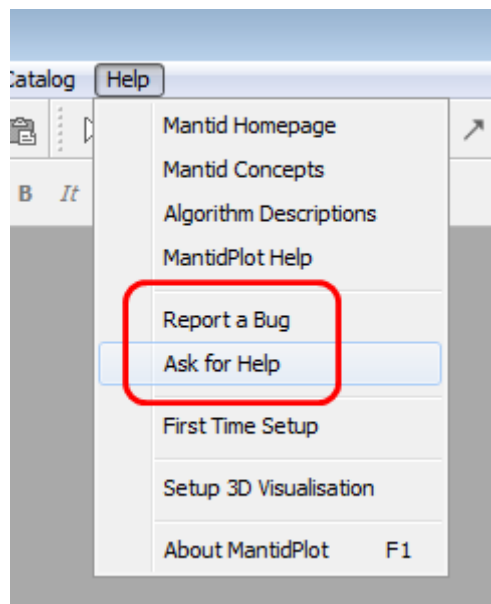
- Not officially supported, but works
 - Windows 10



Windows 10



Mantid Support Forum

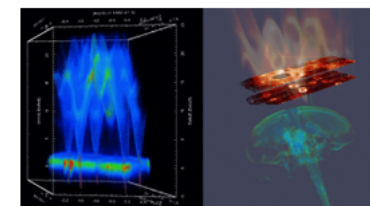
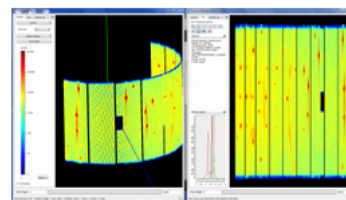
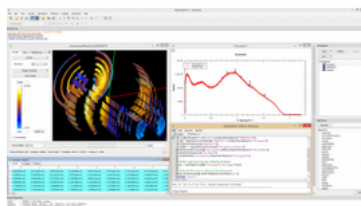


forum.mantidproject.org
help.mantidproject.org

MANTiD



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About Mantid [\[edit\]](#)

The Mantid project provides a framework that supports high-performance computing and visualisation of scientific data.

Mantid has been created to manipulate and analyse neutron scattering and muon spectroscopy data, but could be applied to many other techniques.

The framework is [open source](#) and supported on [multiple target platforms](#) (Windows, Linux, Mac).

Citing Mantid [\[edit\]](#)

O. Arnold, et al., Mantid—Data analysis and visualization package for neutron scattering and μ SR experiments, Nuclear Instruments and Methods in Physics Research Section A, Volume 764, 11 November 2014, Pages 156-166, <http://dx.doi.org/10.1016/j.nima.2014.07.029>

Quick Start Guide [\[edit\]](#)

We have a collection of Mantid training courses that are a great place to start. We run these at facilities as a hands on course (keep an eye on the news section for upcoming courses), but you can also use the course as self-paced training.

- [Mantid Introduction](#)
- [Introduction To Python](#)
- [Python In Mantid](#)
- [Extending Mantid With Python](#)
- [Examples](#)

News [\[edit\]](#)

- 06 Oct 2015
[Version 3.5 is now available](#)
- 21 Sep 2015
[Mantid at CppCon 2015](#)
- 18 Sep 2015
[Mantid is a finalist in the UK IT Industry Computing Awards](#)
- 27 Aug 2015
[Mantid training at ORNL October 26th-27th 2015](#)
- 09 Jul 2015
[Mantid training at ISIS September 21st-23rd 2015](#)

[News Archive](#) | [Help Forum](#) | [Roadmap](#) | [Developer site](#)



Mantid Support Forum

[Sign Up](#)[Log In](#)[all categories](#)[Latest](#)[Top](#)[Categories](#)

Topic	Category	Users	Replies	Views	Activity
📌 Welcome to the Mantid Forums					
The Mantid project provides a framework that supports high-performance computing and visualisation of scientific data. This forum is for users of the software that are looking for help. Other places to look for help are... read more			0	43	Aug 3
Mantid training at ISIS September 21st-23rd 2015	News		2	63	7d
Show Detector Table	General		2	25	7d
Mantid training at ORNL October 26th-27th 2015	News		0	38	19d
Detector position on GEM inst at ISIS	General		1	24	26d
I have changed my IDF but mantid is using a different file	General		1	30	Aug 14
Version 3.4 is now available	News		0	50	Aug 4
Sequential Fit interface	General		0	36	Jul 31
Mantid crashes and does not start any more	Installation		1	38	Jul 30
Will installing another version of Python affect Mantid on Windows	Installation		1	30	Jul 30
Can you change workspace labels in Python?	Python		1	28	Jul 27




Mantid Support Forum


Create New Account




 with Google

 with Facebook

 with Twitter

 with Yahoo

 with GitHub

Email

Never shown to the public

Username

Unique, no spaces, short

Name

Your full name (optional)

Password

At least 8 characters.

Create New Account

Log In

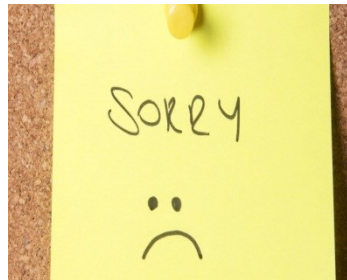


User Interface



Windows Installation

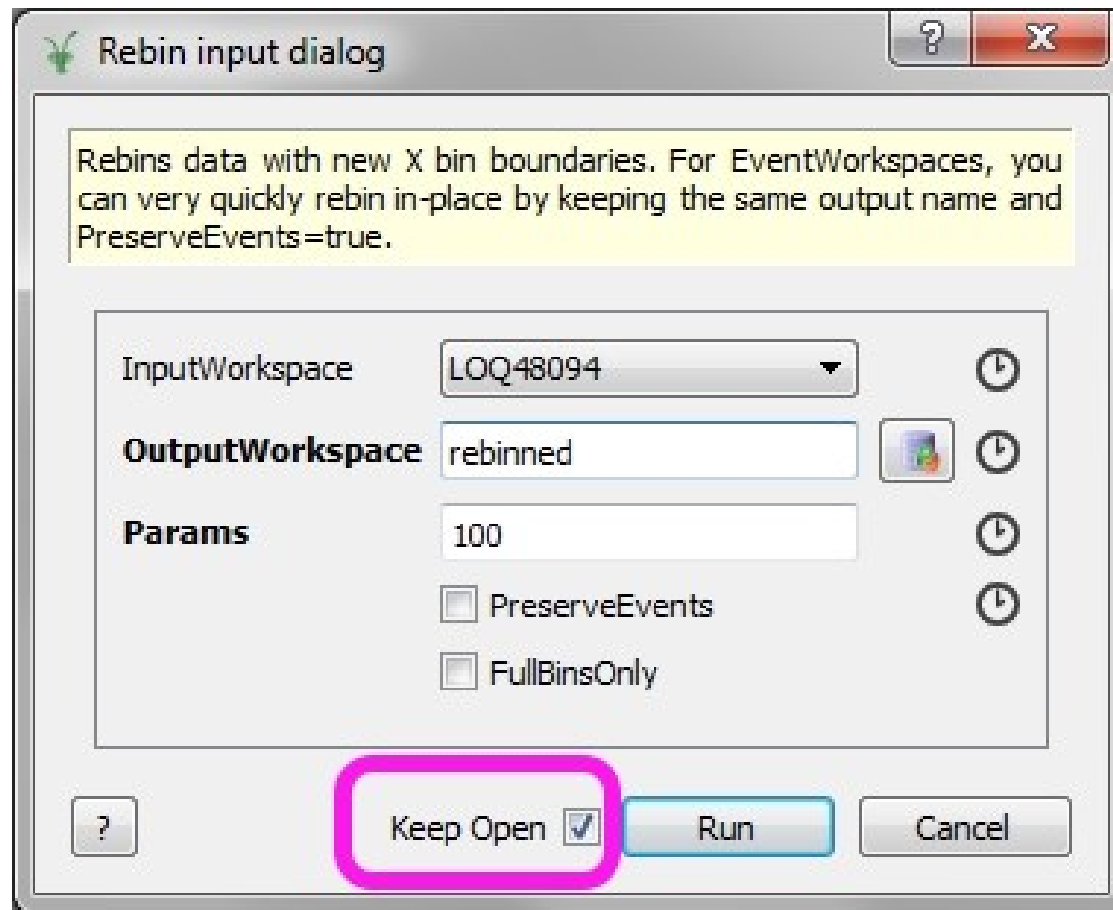
- Each Windows install now self contained
 - Multiple installs without worry of picking up correct libs
- Installer process streamlined
 - Fewer button clicks
 - Progress reports for removing old version
 - Future versions won't have to click 'ok' to start removal



- Shortcuts that were attached to task launcher were broken
 - fix is to simply delete and drag a new one on from desktop



Algorithm Dialogs





Script Window

The screenshot shows a window titled "MantidPlot: Python Window" with a menu bar (File, Edit, Execute, Window, Help) and a tab for "SXD_NaCl.py". The script content is as follows:

```
1 #pylint: disable=invalid-name
2 def reportUnitCell(peaks_ws):
3     latt = peaks_ws.sample().getOrientedLattice()
4     print "-- Unit Cell --"
5     print latt.a()
6     print latt.b()
7     print latt.c()
8     print latt.alpha()
9     print latt.beta()
10    print latt.gamma()
```

The output area shows the following text:

```
-----
Mon 28. Sep 14:07:59 2015: Script execution started.
-----

Niggli cell found from FindUBUsingFFT:
-- Unit Cell --
3.9941636806
3.99365518754
4.00826844429
59.975089371
59.9336161773
60.0428144665
The final result is:
-- Unit Cell --
5.66217987784
5.64251816576
5.65827502489
5.6511104047
```

The status bar at the bottom indicates "Status: Stopped".

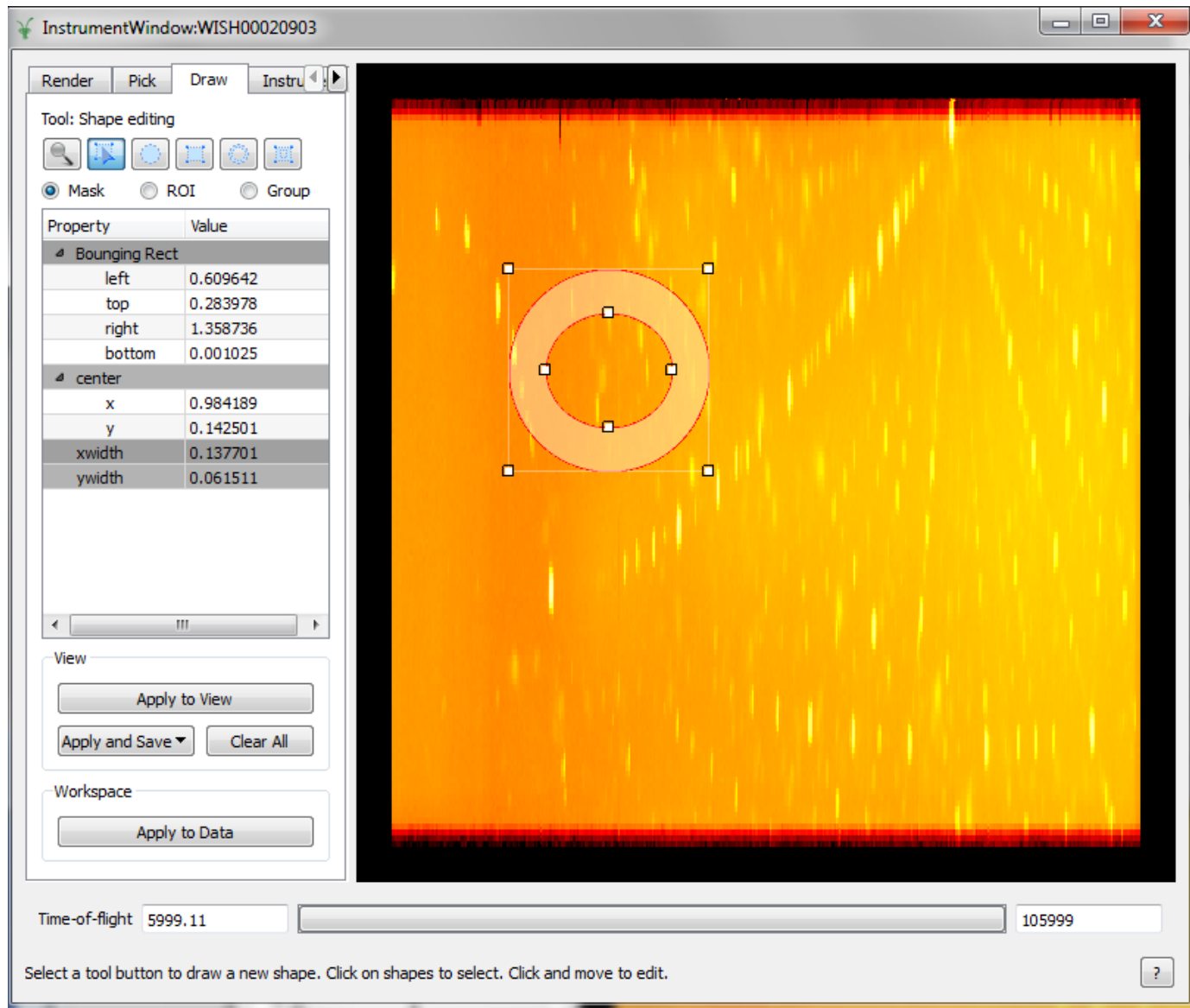


Script Window

- You can now abort scripts!
 - Execute Menu → Abort
 - Or “Ctrl+D” shortcut
- Warning – it’s a request
 - It can take a moments to satisfy
 - If an algorithm doesn’t cancel effectively → tell us

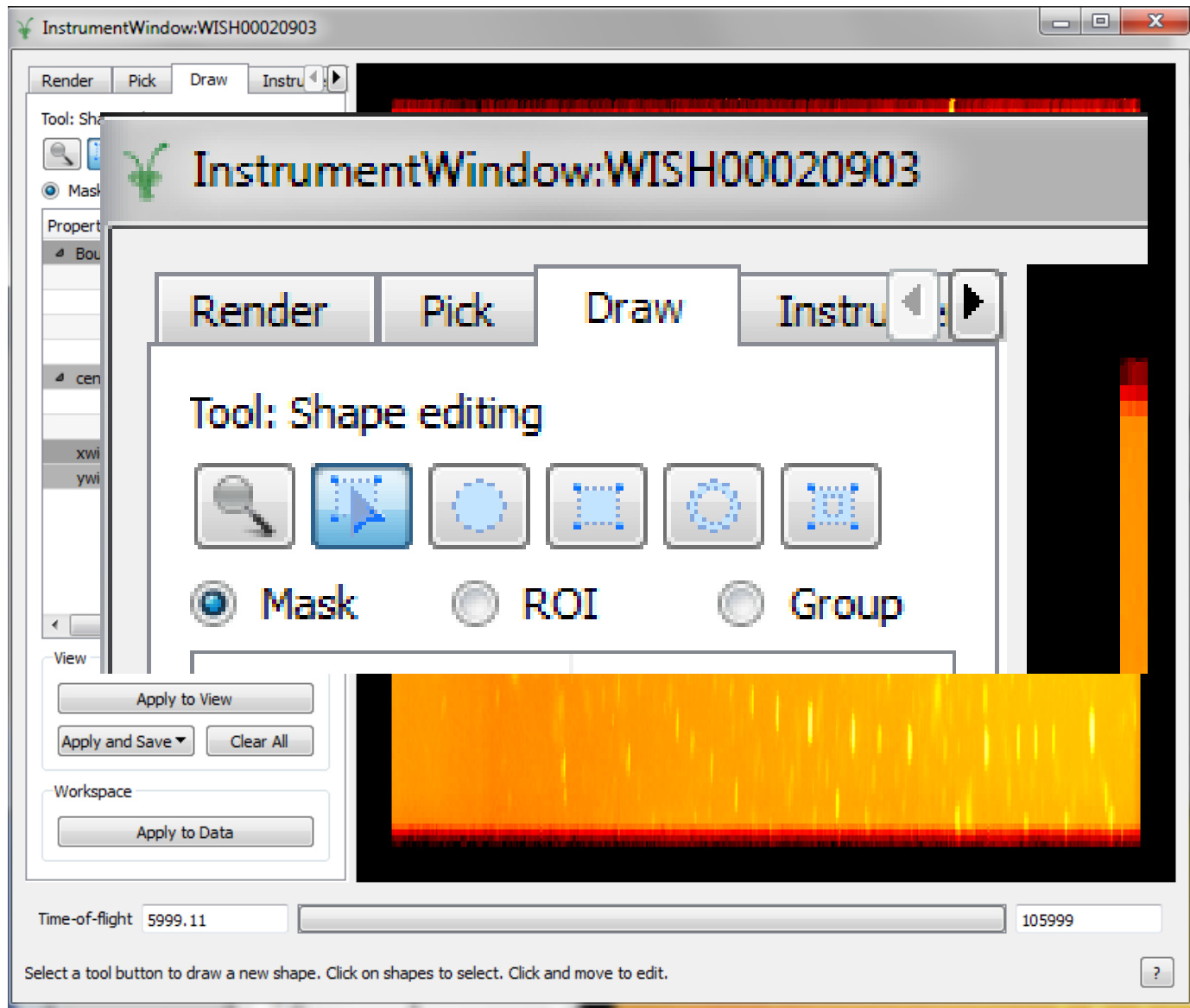


Instrument View



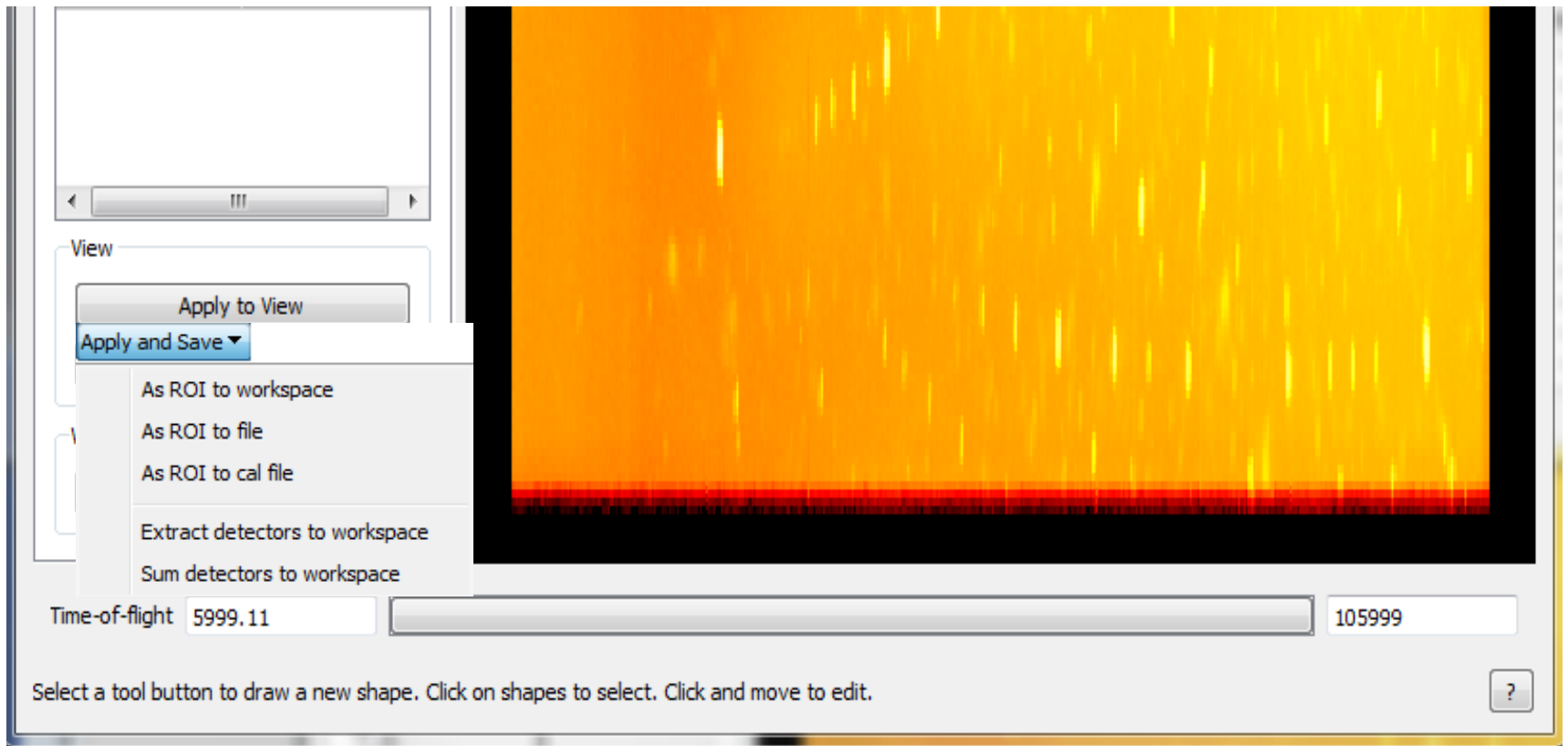


Instrument View



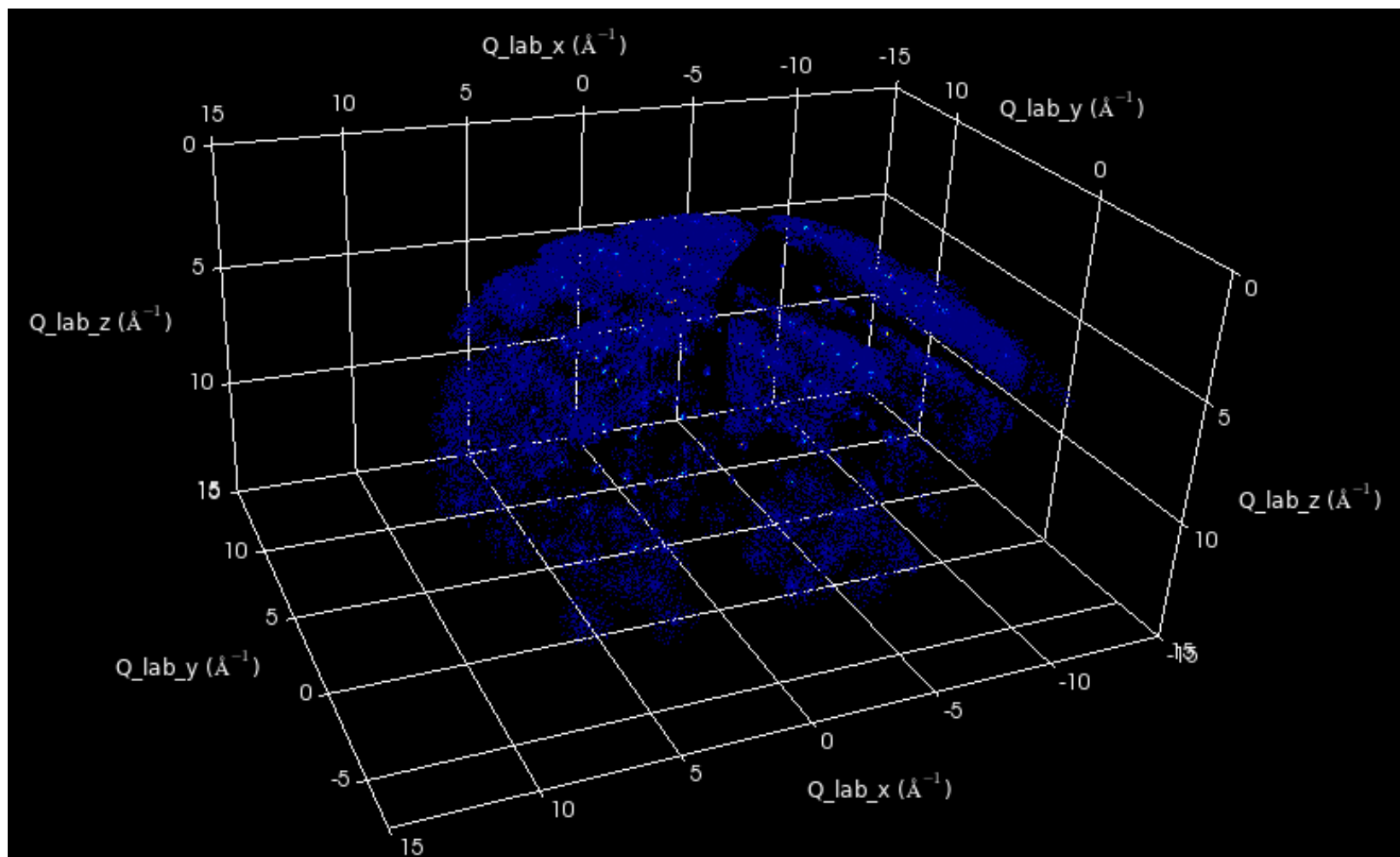


Instrument View





VSI





Framework



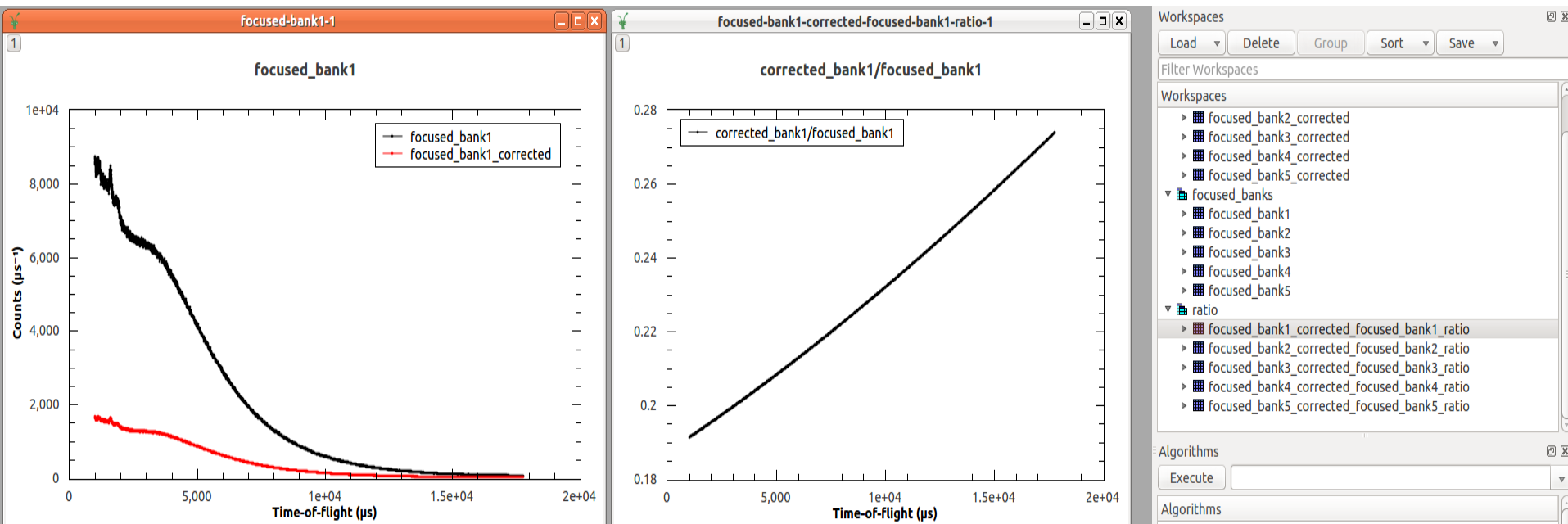
Multiple Scattering

- New algorithm for corrections due to absorption and multiple scattering - `MayersSampleCorrection`
 - Based on J. Mayers OpenGenie correct routine
 - Cylindrical sample, elastic scattering
 - Multiple scattering requires isotropic scatterer
 - Multiple scattering correction is optional
- <http://docs.mantidproject.org/nightly/algorithms/MayersSampleCorrection-v1.html>
- Needs more widespread testing!



Multiple Scattering

- Example: corrected data & ratio for bank1 of POLARIS vanadium run



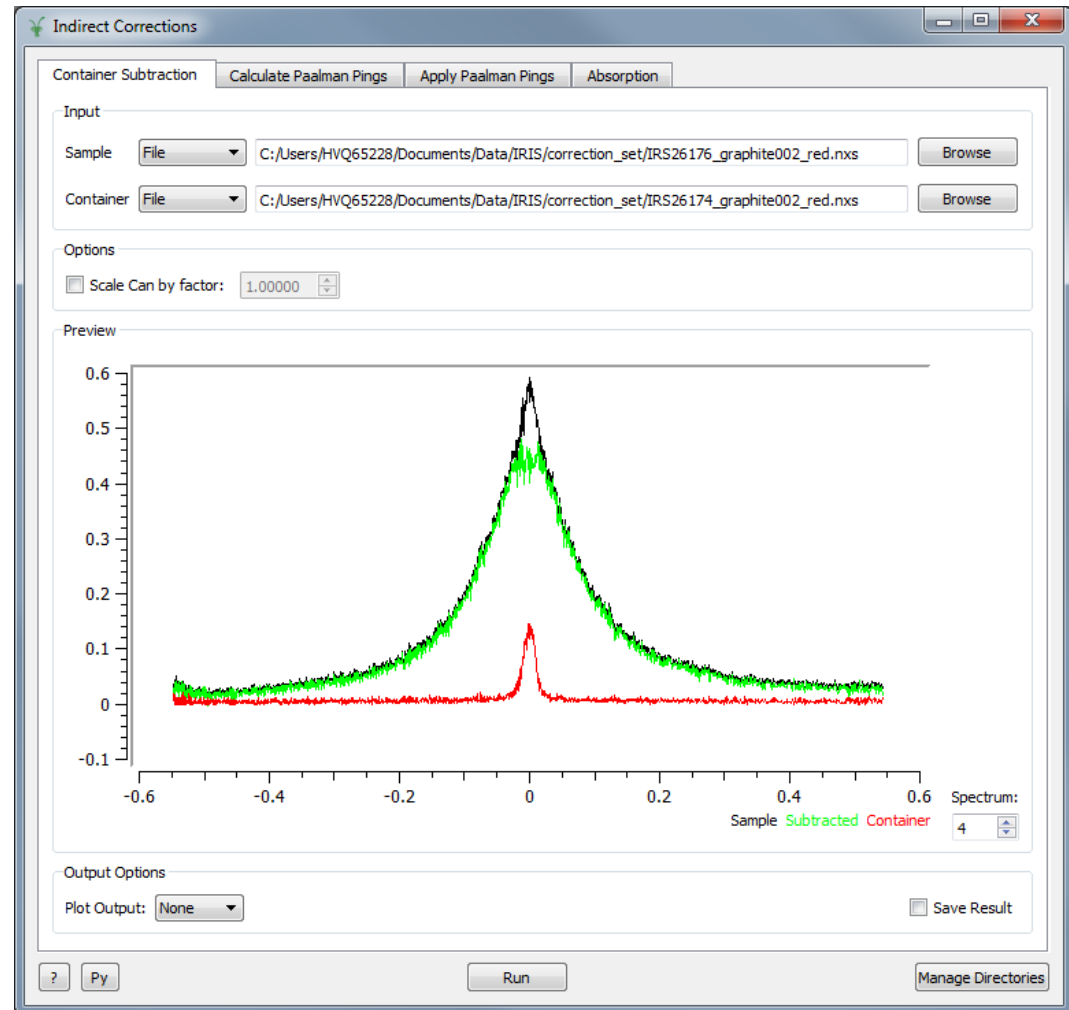


Indirect Inelastic



Corrections

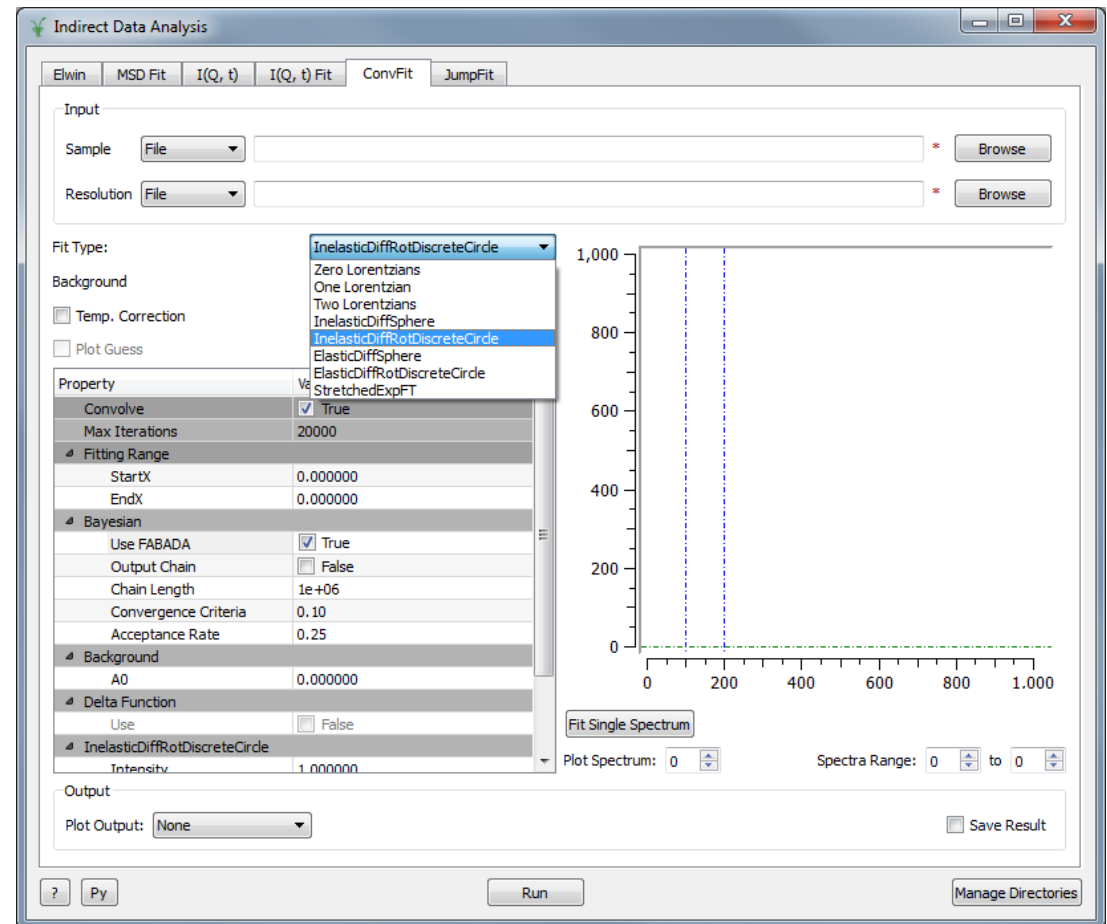
- New interface
 - Interfaces > Indirect > Corrections
- Container Subtraction
 - Simple interface that only subtracts the container





Data Analysis

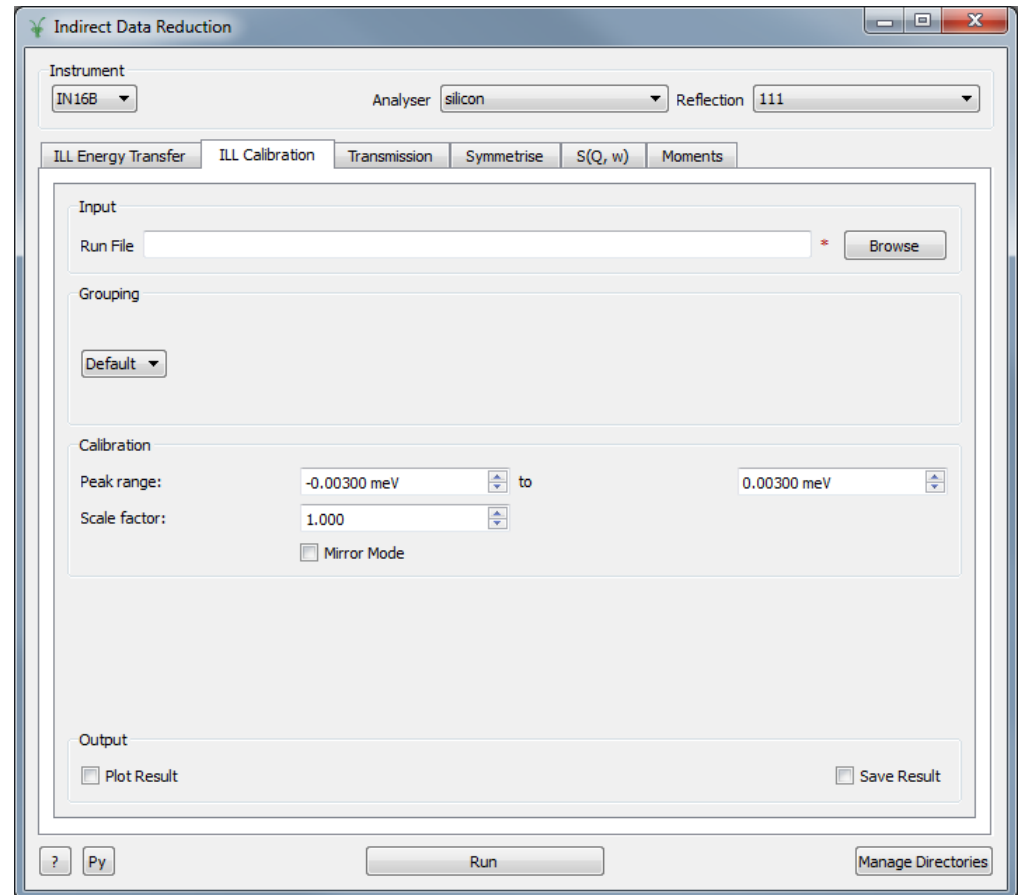
- ConvFit
 - Support for Quasi elastic fit functions
 - Mantid Algorithm
- Bayesian Analysis
 - FABADA in ConvFit and I(Q, t) Fit





Data Reduction

- Facility Support for the ILL
- ILL Calibration tab
 - IN16B





Simulation

- nMOLDYN
 - Support for nMOLDYN 4
- Density Of states
 - DOS spectra output for TOSCA comparison

The screenshot shows the 'Indirect Simulation' dialog box with three tabs: 'MolDyn', 'Sassena', and 'DensityOfStates'. The 'MolDyn' tab is active. It contains the following sections:

- nMOLDYN**:
 - Version: A dropdown menu with options 3 and 4; option 4 is selected.
 - Data: A text input field with a red asterisk and a 'Browse' button.
 - Function Names: A text input field.
- Options**:
 - ☒ Crop Max Energy: A numeric input field set to 10.00000 meV.
 - ☒ Symmetrise Energy.
- Instrument Resolution**:
 - ☐ Use Instrument Resolution.
 - Resolution: A dropdown menu set to 'File', a text input field, a red asterisk, and a 'Browse' button.
- Output Options**:
 - Plot Result: A dropdown menu set to 'None'.
 - ☐ Save Result.

At the bottom of the dialog are three buttons: a help button (question mark), a 'Run' button, and a 'Manage Directories' button.

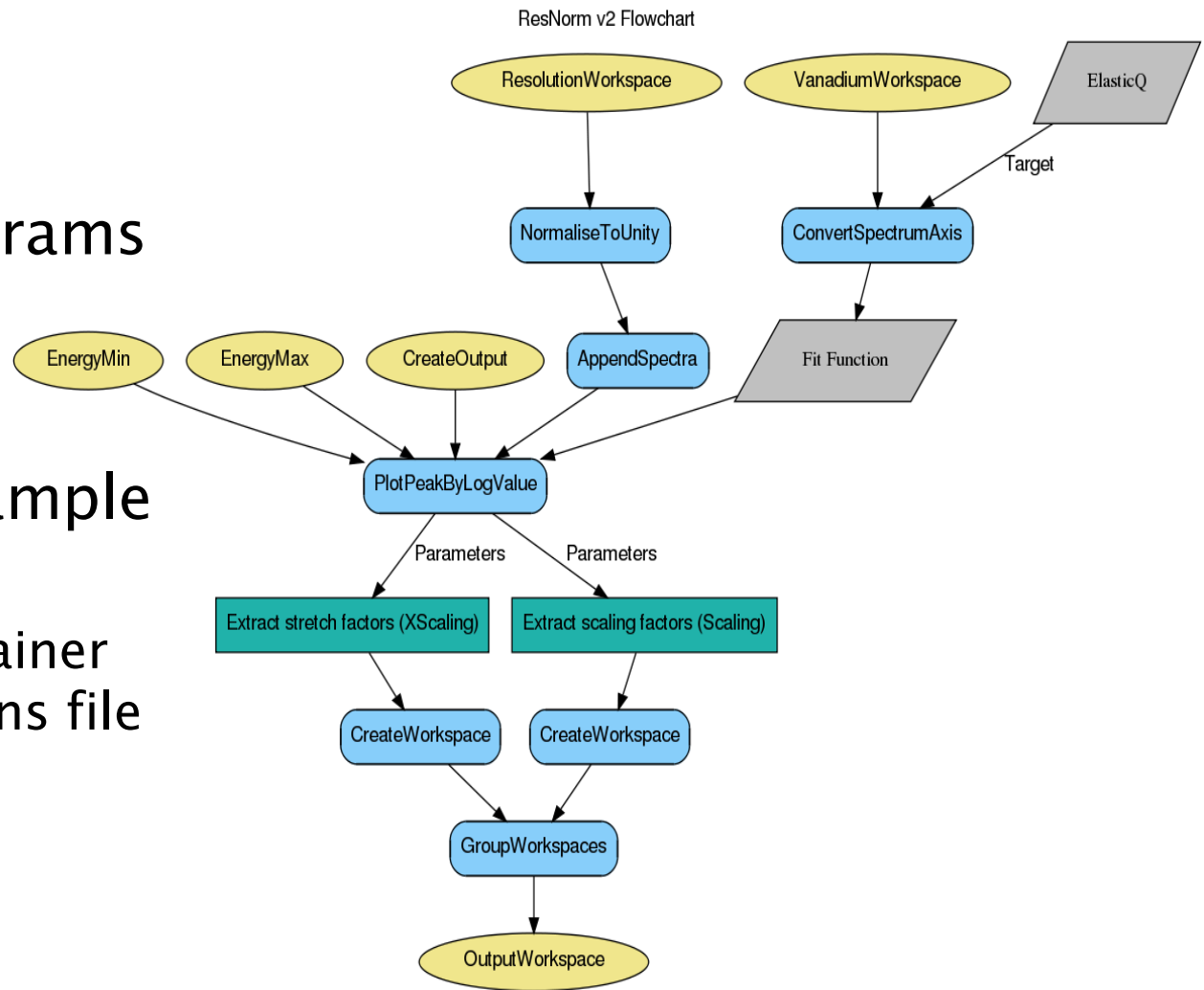


Documentation

- Workflow diagrams

- Corrections Sample logs

- Sample, Container and Corrections file

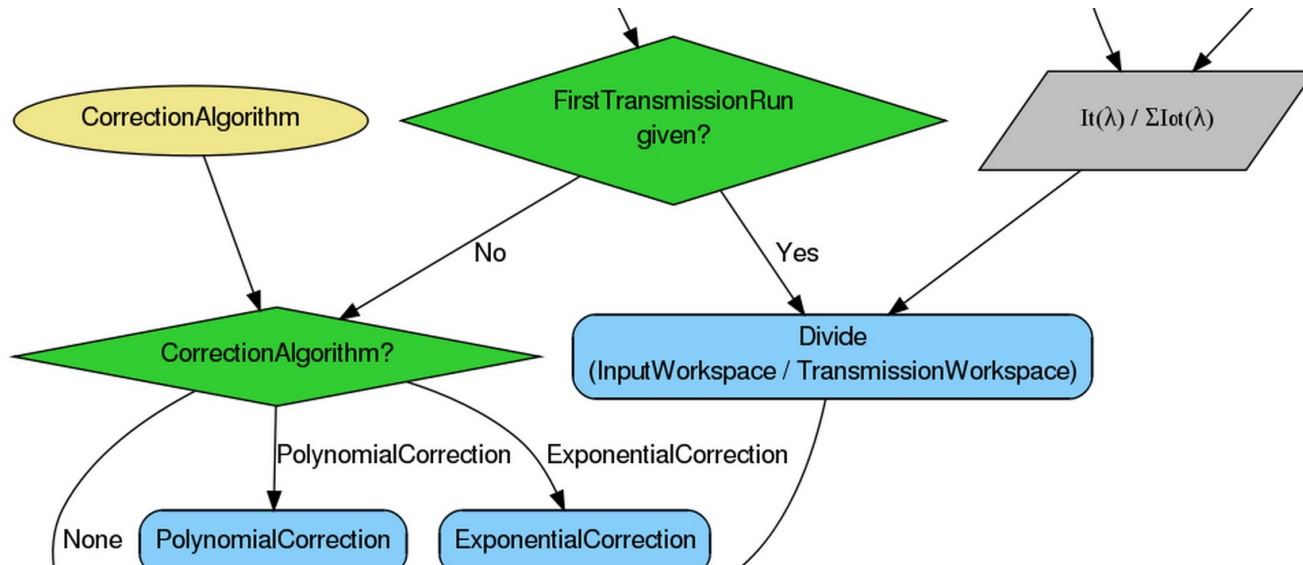




Reflectometry



Transmission Correction



Polynomial Corrections

CorrectionAlgorithm ☒ None ☐ AutoDetect ☐ PolynomialCorrection ☐ ExponentialCorrection

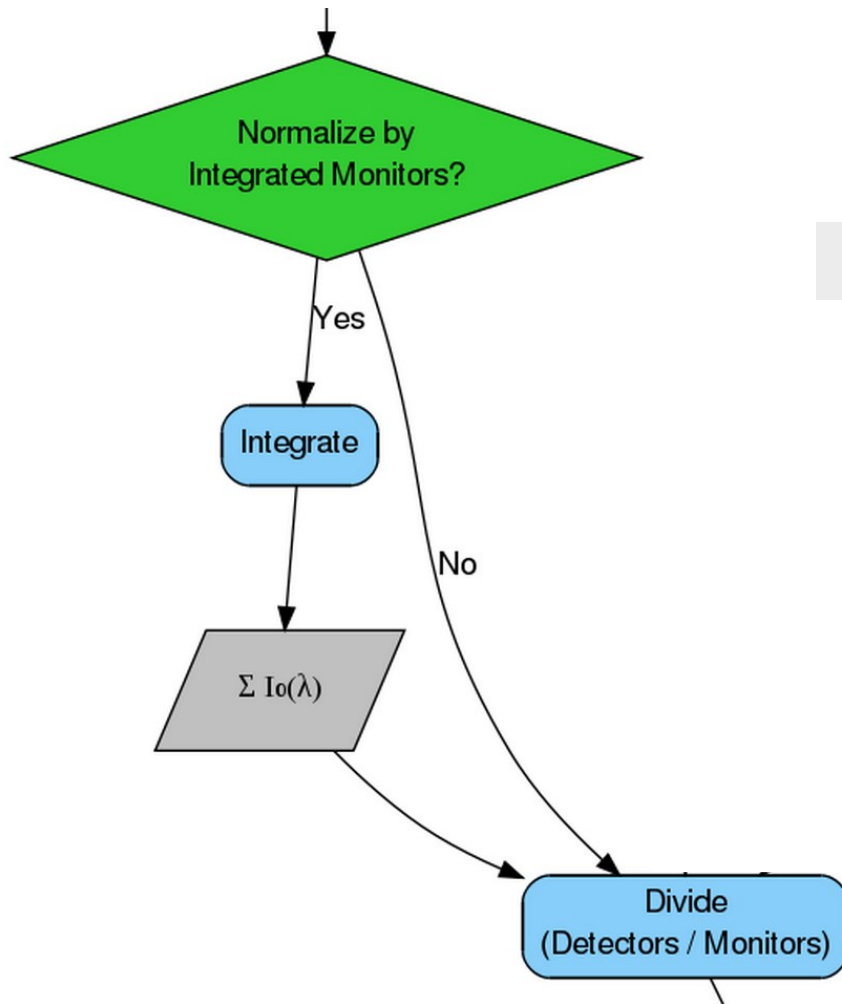
Polynomial

C0

C1



Monitor Normalization



☒ NormalizeByIntegratedMonitors



ConvertToReflectometryQ (SofQW)

InputWorkspace input

OutputDimensions Q (lab frame)

Method NormalisedPolygon

IncidentTheta 0.44

- Convert to Q_x, Q_z
- Convert to K_i, K_f
- Convert to $P_i - P_f, P_i + P_f$.

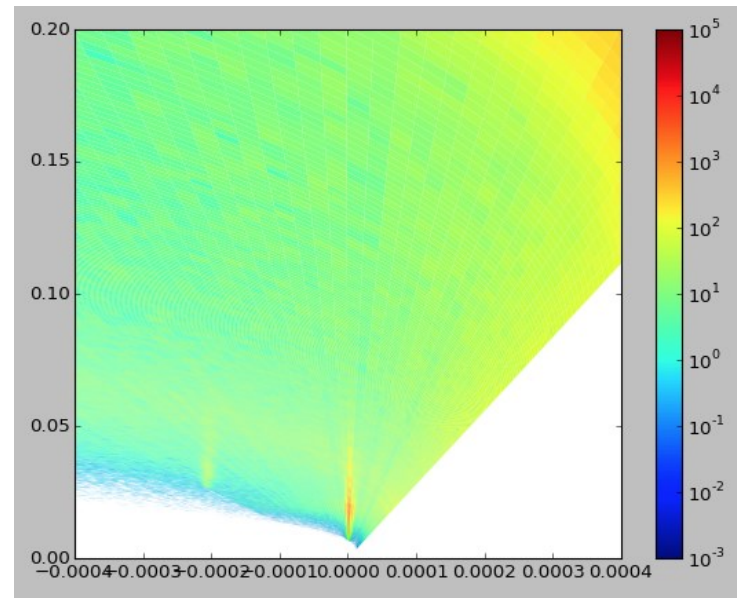
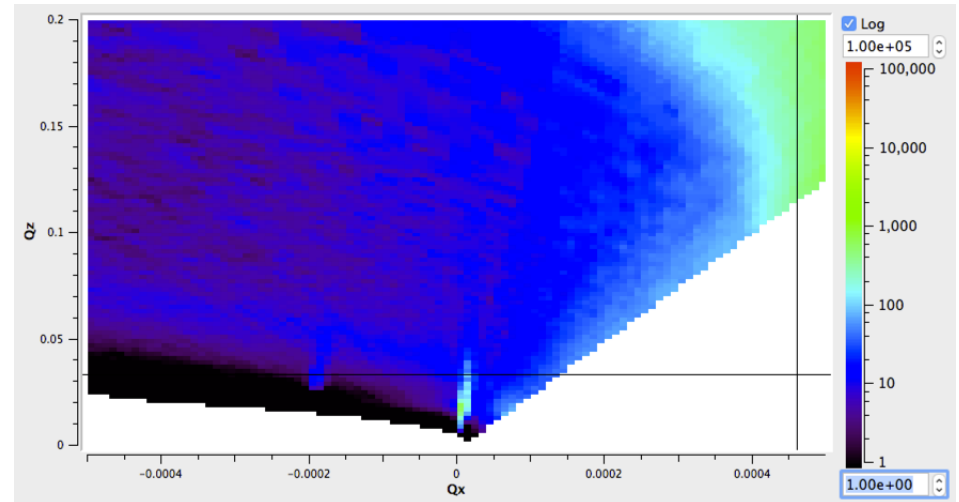
where

$$Q_x = \frac{2\pi}{\lambda}(\cos\theta_f - \cos\theta_i)$$

$$Q_z = \frac{2\pi}{\lambda}(\sin\theta_f + \sin\theta_i)$$

$$K_i = \frac{2\pi}{\lambda}\sin\theta_i$$

$$K_f = \frac{2\pi}{\lambda}\sin\theta_f$$





Electronic Notebooks

Reflectometry Edit

Search Runs
Instrument: INTER
Investigation Id:
Search

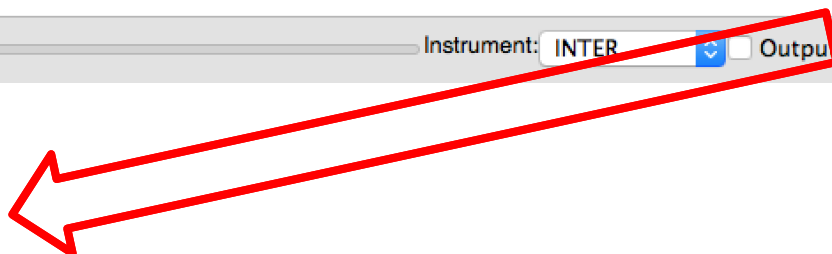
Process Runs

	Run(s)	Angle	Transmission Run(s)	Q min	Q max	dQ/Q	Scale	Group	Options
1	13460	0.5	13463,13464	0.01	0.06	0.04	1	1	
2	13462	2.3	13463,13464	0.035	0.3	0.04	1	1	
3	13469	0.7	13463,13464	0.01	0.06	0.04	1	2	
4	13470	2.3	13463,13464	0.035	0.3	0.04	1	2	

Transfer

Instrument: INTER Output Notebook Process

Output Notebook Process

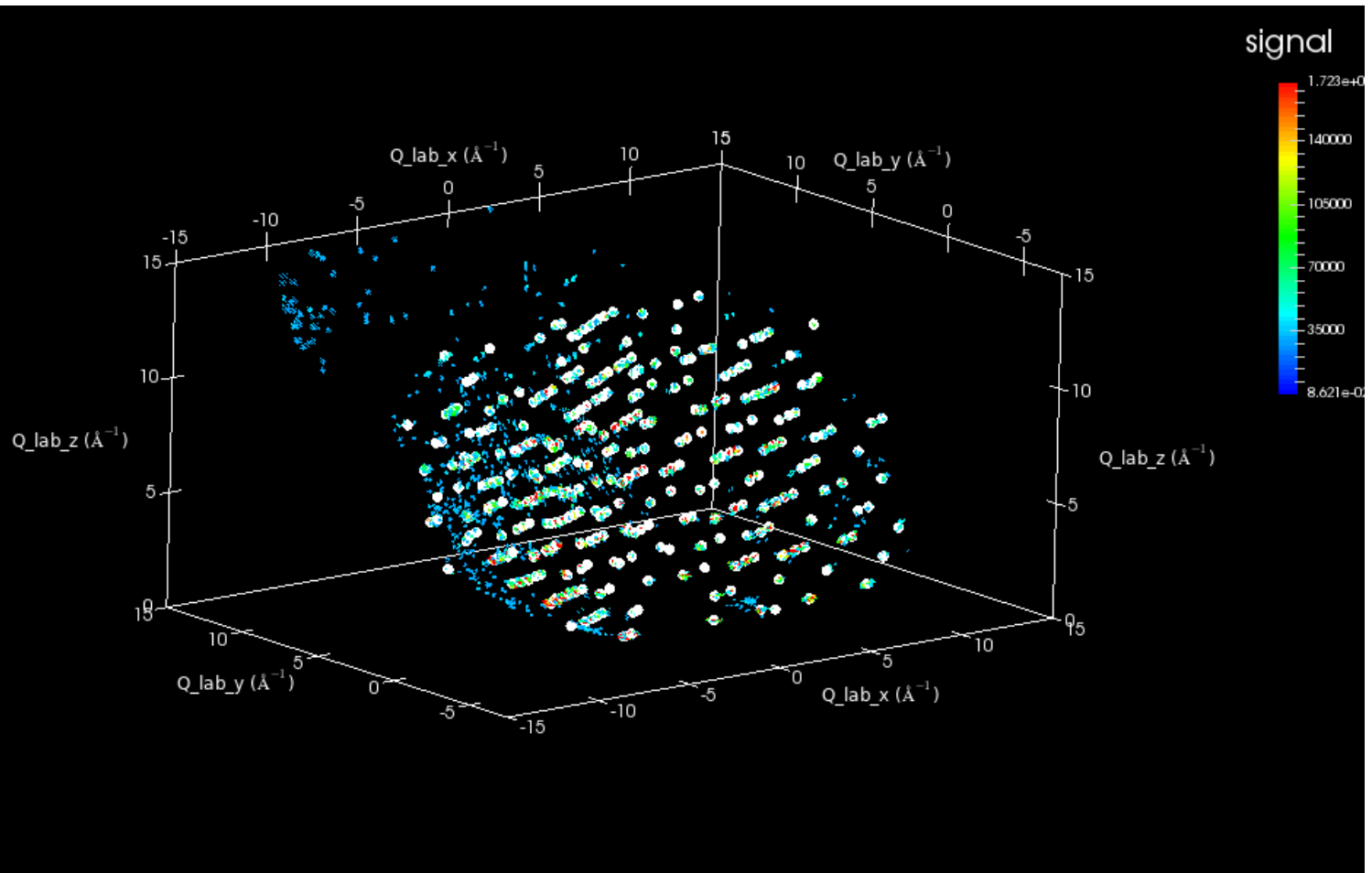




Diffraction

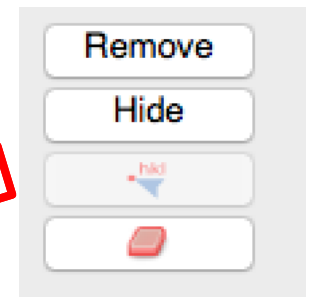
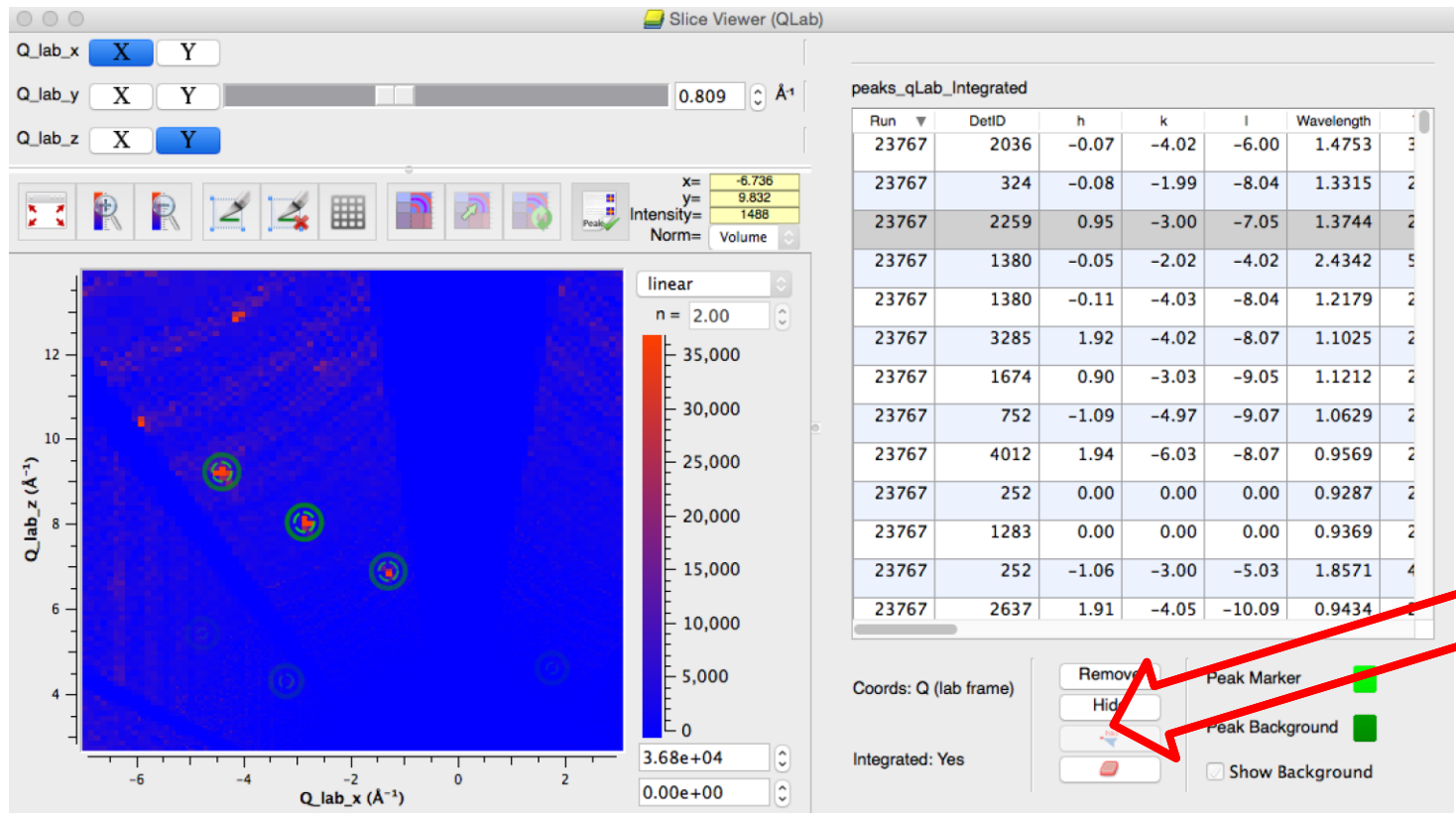


3D Visualisation





PeaksViewer Interactive Modes





Other Diffraction Improvements

- Major bug fix for BinMD and SliceMD
- “Group” has been exposed to python
- Other improvements to “SpaceGroup” and “PointGroup” (see documentation)
- TransposeMD and ReplicateMD added
- New Engineering UI for calibration and focusing
- Migration of Powder scripts to Mantid 3.5



SANS



Extended Transmission Settings (Reduction Settings Tab)

Transmission Settings

☐ M3☐ M4☒ Radius☒ ROI files

Shift:

2

ROI1.XML,ROI2.XML

Masking files:

MASK1.XML

User File Commands:

TRANS/RADIUS=r

TRANS/ROI=roi_mask.xml

TRANS/MASK=mask.xml

Overlay added event workspaces (Add Runs Tab)

Histogram binning (when adding event data):

Save as event data

☒ OverlayEventWorkspaces

Additional Time Shifts:



- Inflate zero-errors

Save

Filename:

Formats: ☒ Nexus ☐ NIST Qxy ☒ CanSAS ☐ RKH ☐ CSV

☒ Inflate Zero Error

- Support for loading multi-period event data
- Individual User Files in Batch mode

CSV File

	Sans Sample	s Sa	t Sa	ns C	ns C	ct C	Output Name	User File
1	92053						iteration_individual_user_file_1	user_file_1.txt
2	92053						iteration_individual_user_file_2	user_file_2.txt
3	92053						iteration_individual_user_file_3	user_file_3.txt

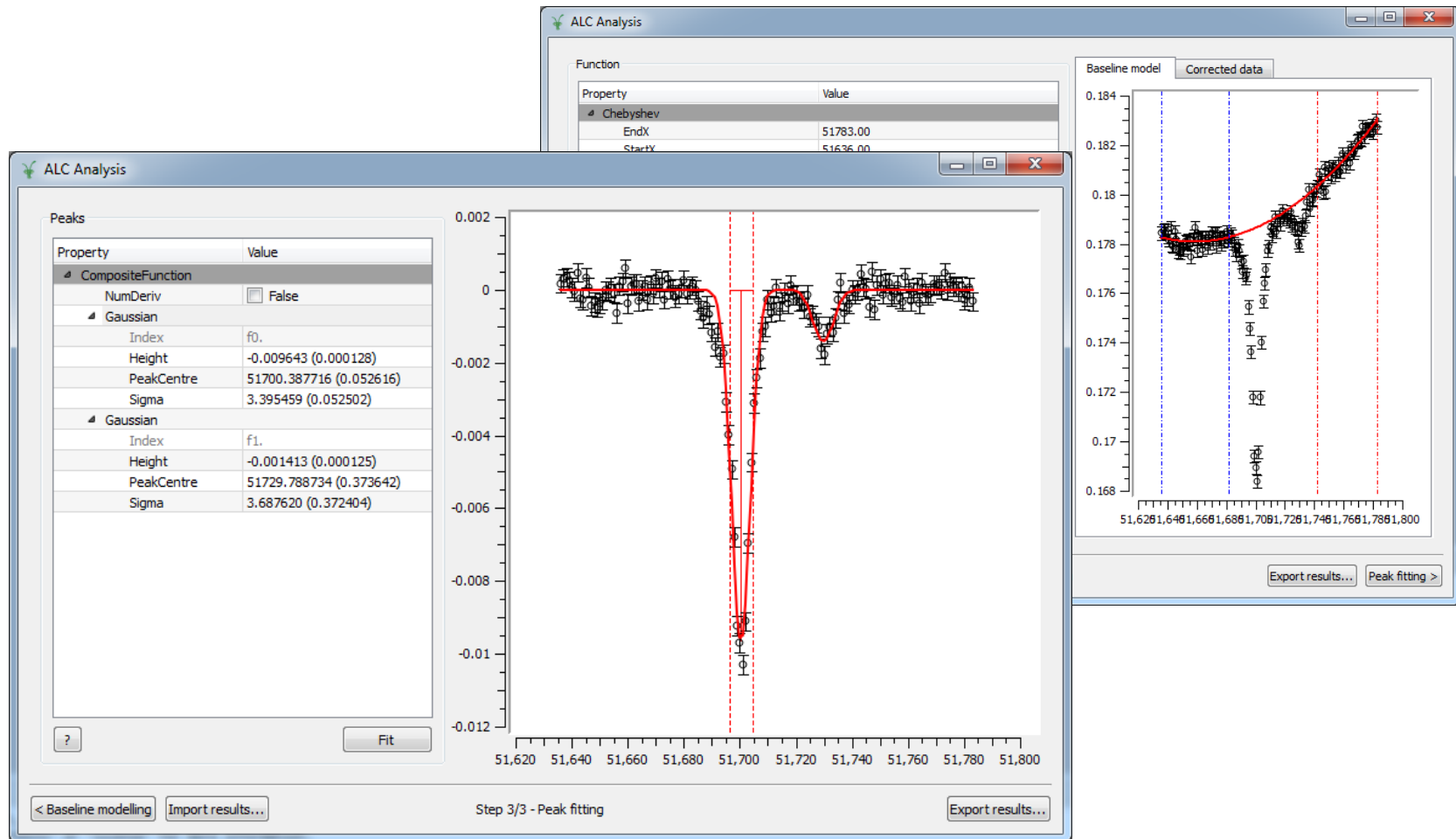


Muon



ALC

- Error bars



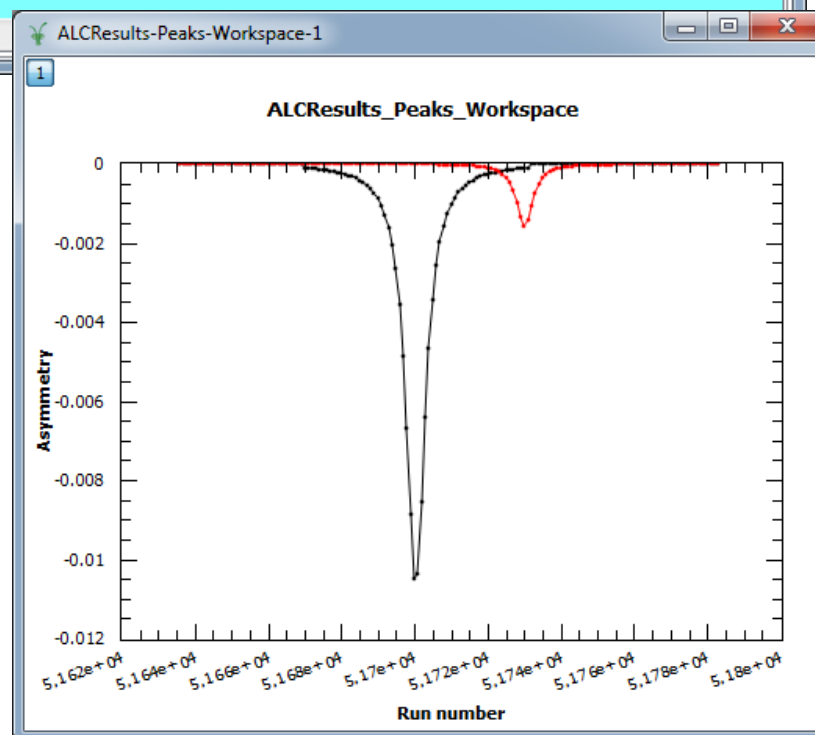
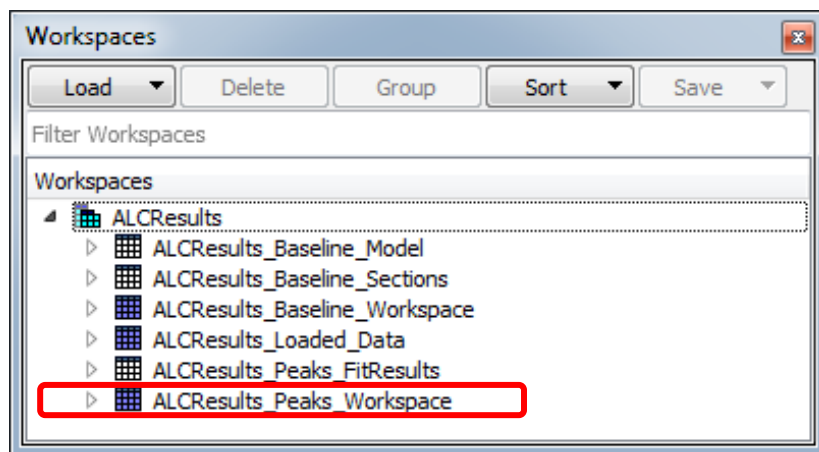


ALC

- Peaks exported as separate spectra

ALCResults_Peaks_Workspace

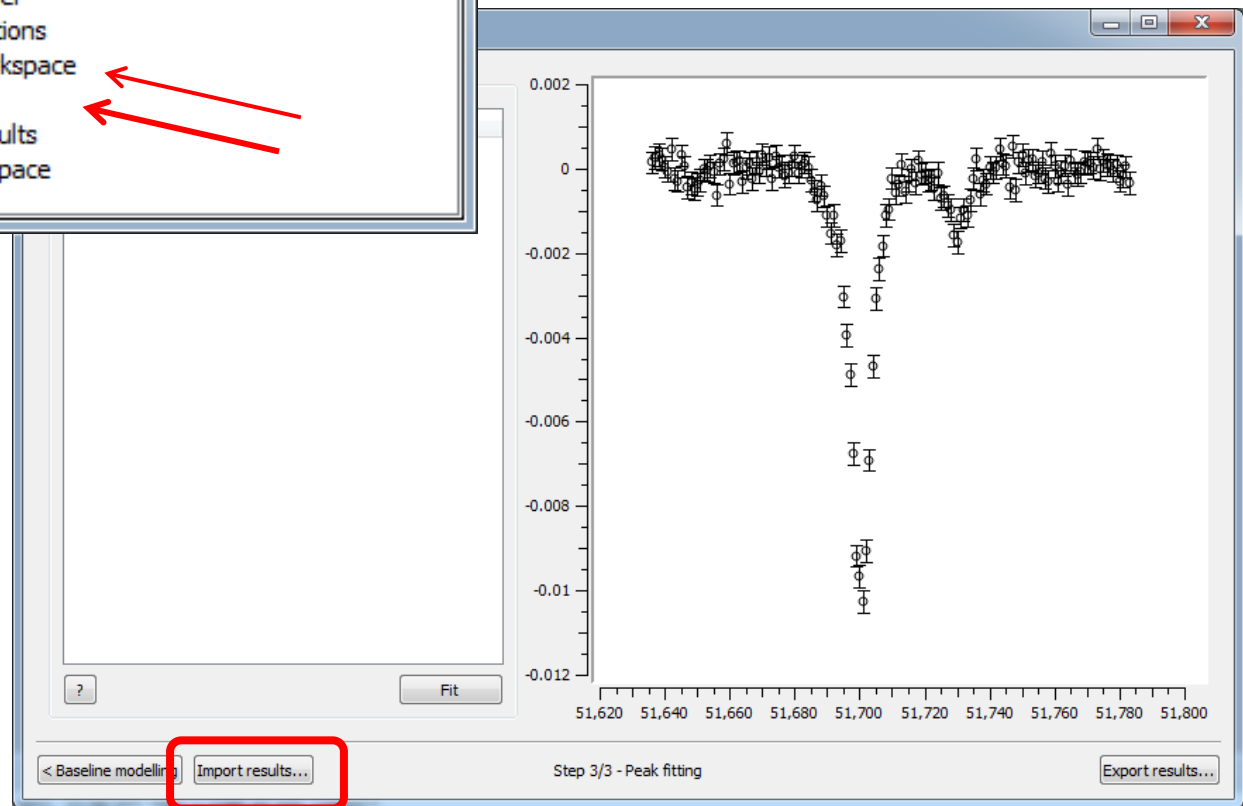
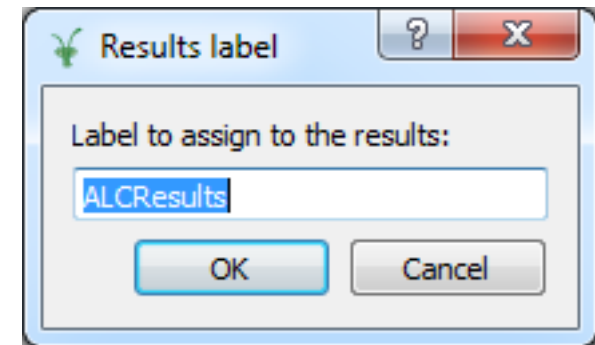
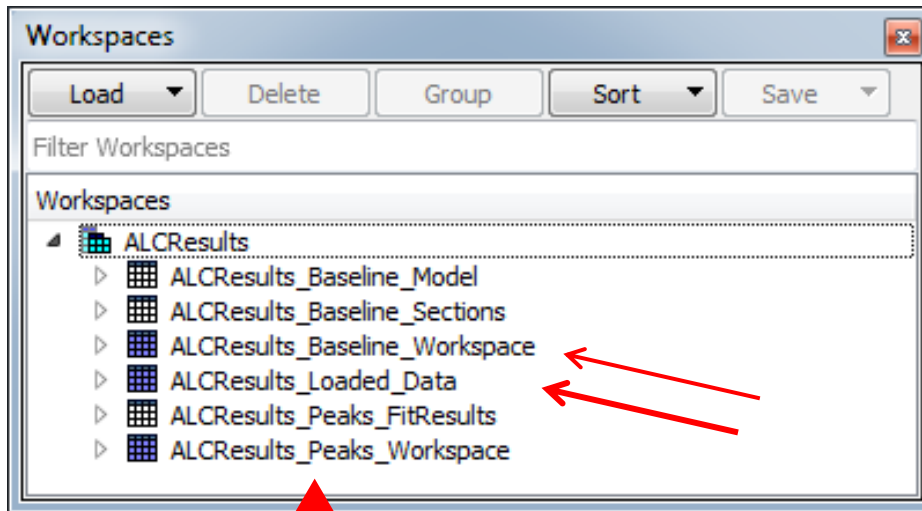
Y values	X values	Errors						
	0	1	2	3	4	5	6	
	51636	51637	51638	51639	51640	51641	51642	
Data	1.729947e-04	2.908773e-04	3.520181e-04	2.519578e-04	6.268262e-05	-4.075070e-05	4.725842e-04	-2.2
Calc	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.00
Diff	1.729947e-04	2.908773e-04	3.520181e-04	2.519578e-04	6.268262e-05	-4.075070e-05	4.725842e-04	-2.2
Lorentzian	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.00
Lorentzian	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00	0.00





ALC

- Import results



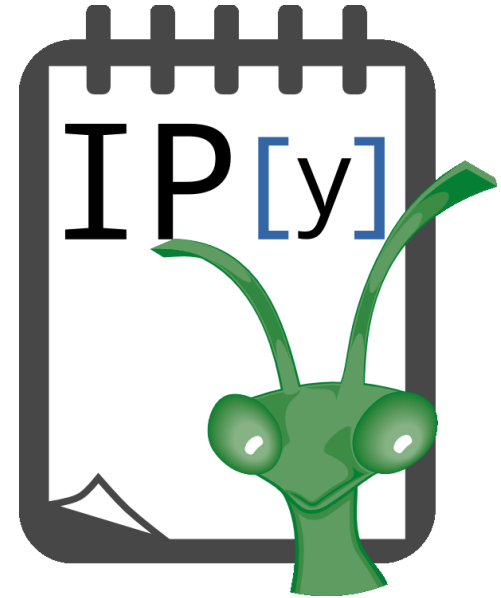


IPython Notebooks



IPython Notebooks

- Record results, analysis, notes
 - Electronic laboratory notebook
- Features:
 - User editable
 - Cross-platform
 - Simple to re-execute
 - Annotation, including equations and tables
 - Inline figures using matplotlib
 - Printable or easily export to PDF
 - Use Mantid's Python API
- Now adding specific support to MantidPlot





IPython Notebooks

- Notebooks generated in two places:
 - GenerateIPythonNotebook algorithm
 - ISIS Reflectometry (Polref) interface

Demo



Next Release



Release v3.6

- Planned Release Date: End Jan/ Early Feb 2015

Mantid Scientific Steering Committee

- ORNL
- Most likely dates 20-21st January



Thank you



mantid