

Mantid Release Presentation

Release 3.3
ISIS



What is this meeting

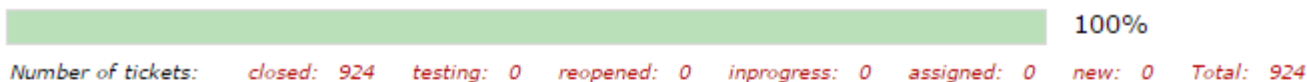
- Release 3.3
 - Released on Monday 19th January
 - Present the changes and improvements
 - Focus on Autoreduction
 - What's coming next



The Mantid Roadmap

Milestone: Release 3.3

Completed 46 hours ago (19/01/15 11:37:23)



Code Freeze: 6-Dec

Beta Testing: 16-Dec to 9-Jan

Headline Tickets:

Diffraction component tickets:

#8930 Fix rectangular detector issues

Framework component tickets:

#8915 GUI design guidelines

#8918 Algorithm naming conventions/standards

#8920 Load performance HDF5

#8924 Repo. for instrument files

#8945 Measure loading performance for large files and optimize

#9105 New MD normalization framework

Python API component tickets:

#8912 Python Command Line interface improvements

Reflectometry component tickets:

#8927 Verification of the ISIS quick scripts (with liquids)

#9295 Artur GUI working with Liquids (outside of mantid if necessary)

#10502 Use Mantid with IPython Notebook

User Interface component tickets:

#8911 MultiDataFitting

#10639 Plotting: Optionally plot counts/width



Training Courses

- Dates
 - Neutron Training Course
 - Should we offer another run before startup?
- To Book
 - Email: nick.draper@stfc.ac.uk
 - More details at www.mantidproject.org





Supported Platforms

- Staying the same

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



OS X Mountain Lion



- Limited support for

- Windows 8 64 bit
- Fedora 20
- RHEL 7 64bit



Windows 8



- No Longer supported

- Ubuntu 12.04 64 bit



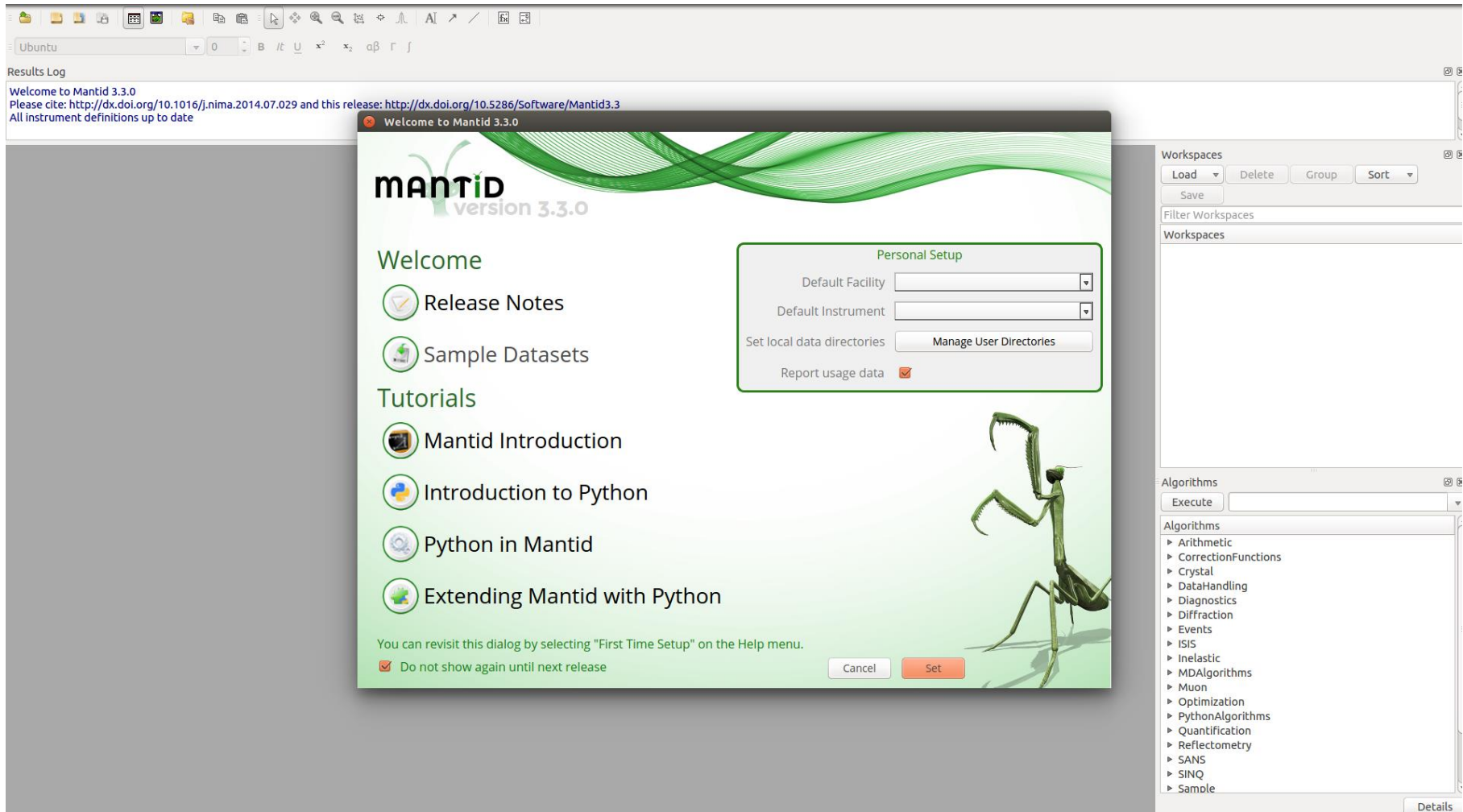


User Interface



Artwork & Startup

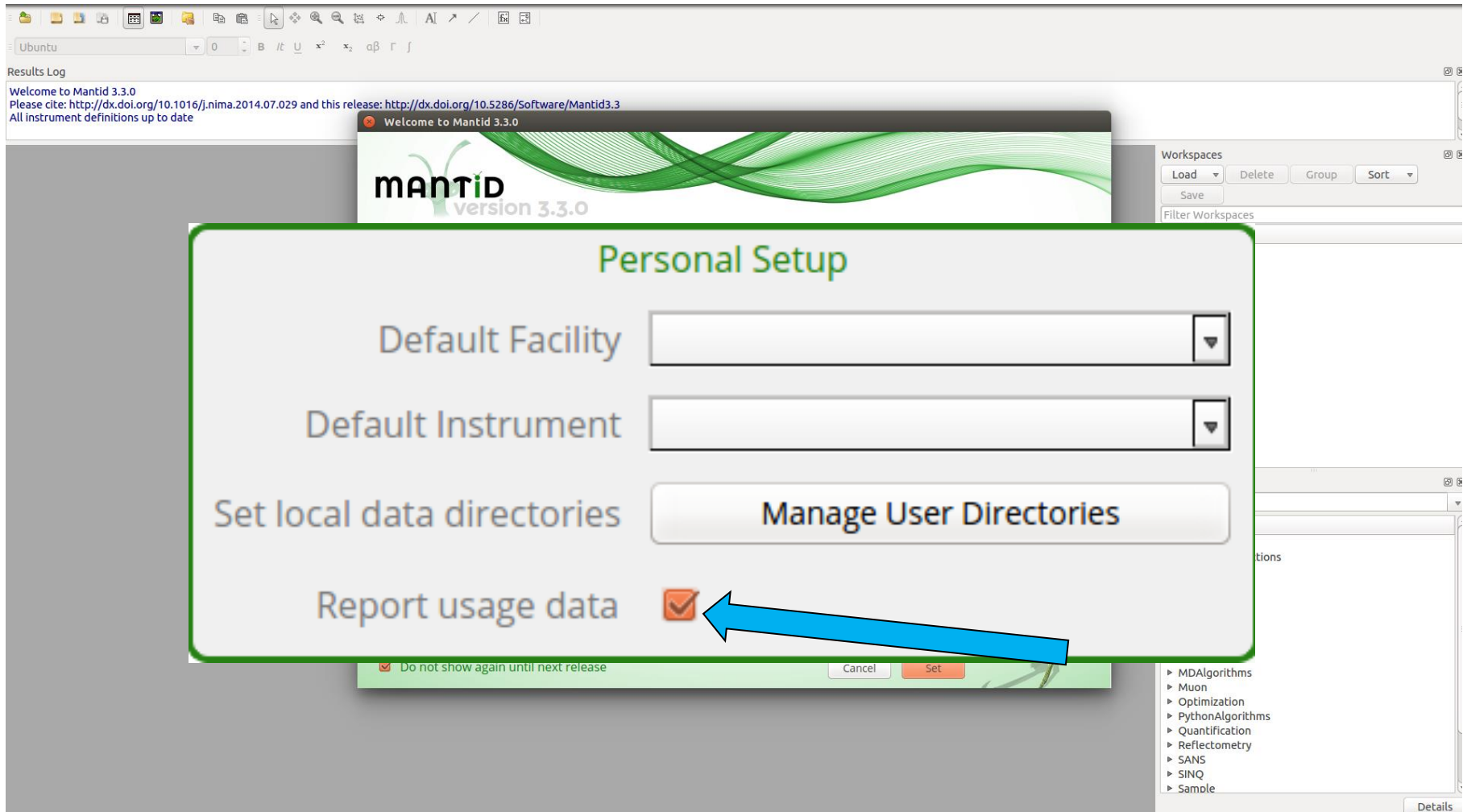
- New artwork provided by ORNL graphics team





Artwork & Startup

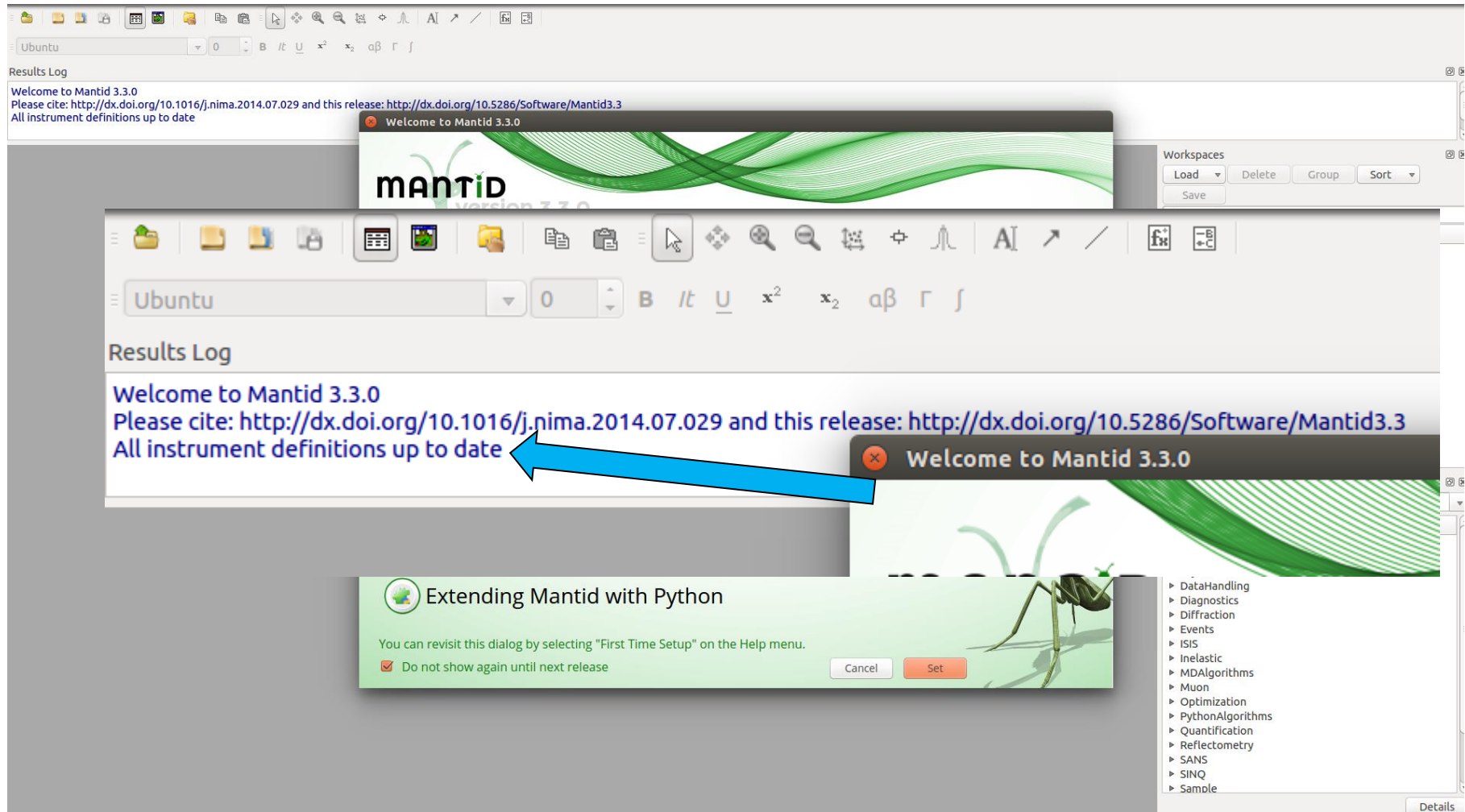
- New artwork provided by ORNL graphics team





Artwork & Startup

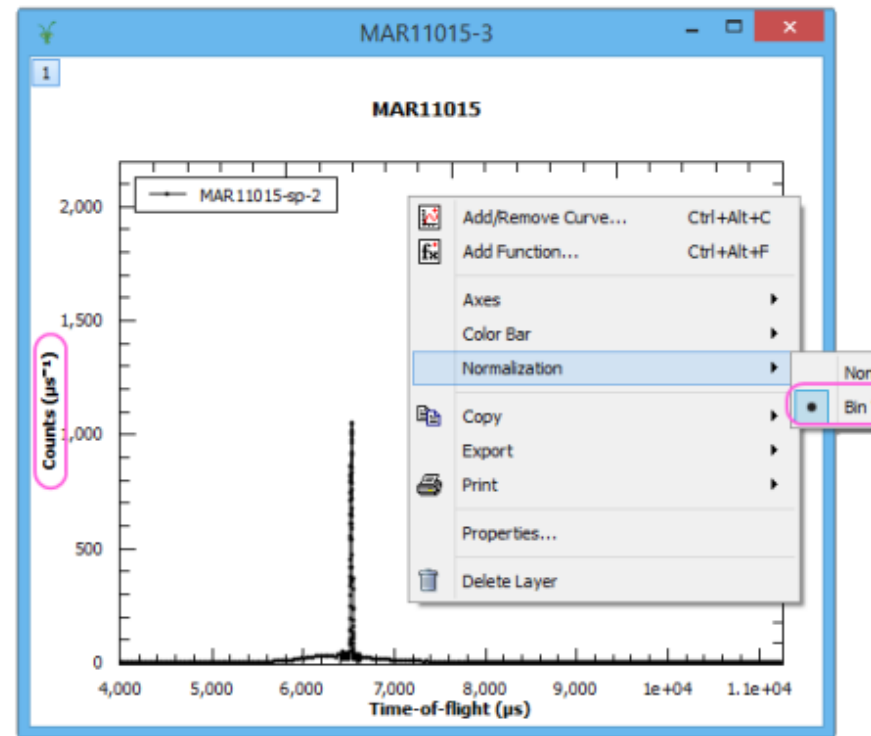
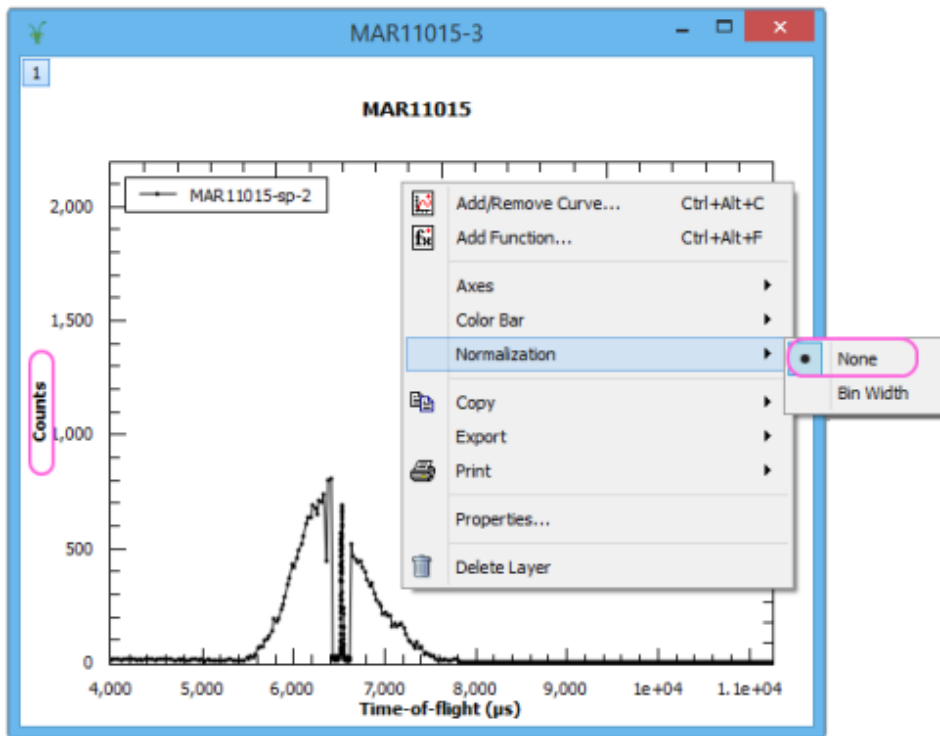
- New artwork provided by ORNL graphics team





Histogram Plots

- Histogram plots are now normalised to bin width by default
- Data is **not** altered





Histogram Plots

2D Plots

Options Axes Curves Ticks Fonts Print

- ☒ Autoscaling
- ☒ Show Title
- ☐ Canvas Frame
- ☒ Normalize histogram to bin width
- ☒ Scale Fonts
- ☒ Antialiasing
- ☐ Fixed aspect ratio on window resize

Margin: 0

☐ Do not resize layers when window size changes

☐ Disable in-place editing

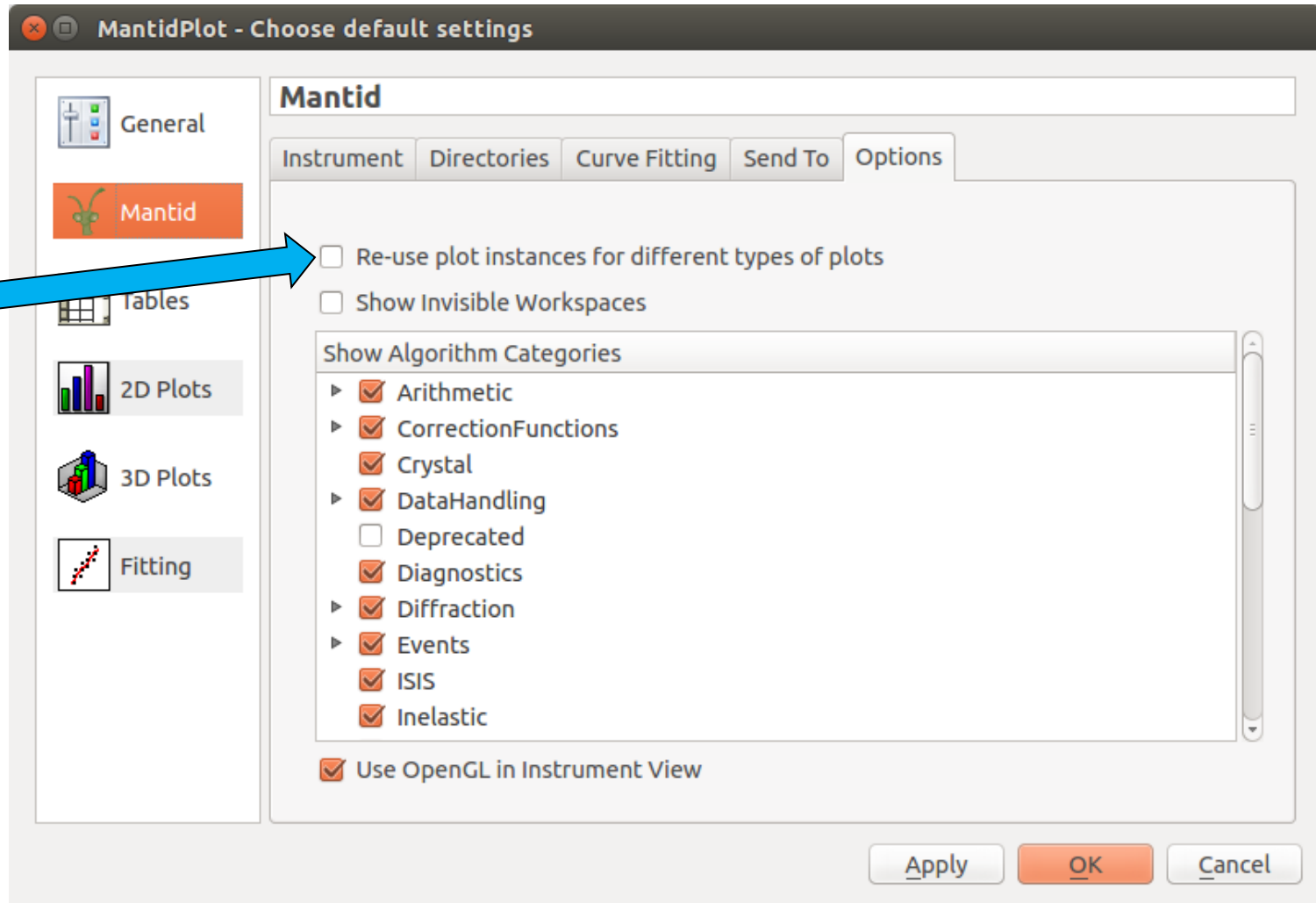
Buttons: Apply, OK, Cancel

Left Plot Y-axis: Counts

Right Plot X-axis: Bin V



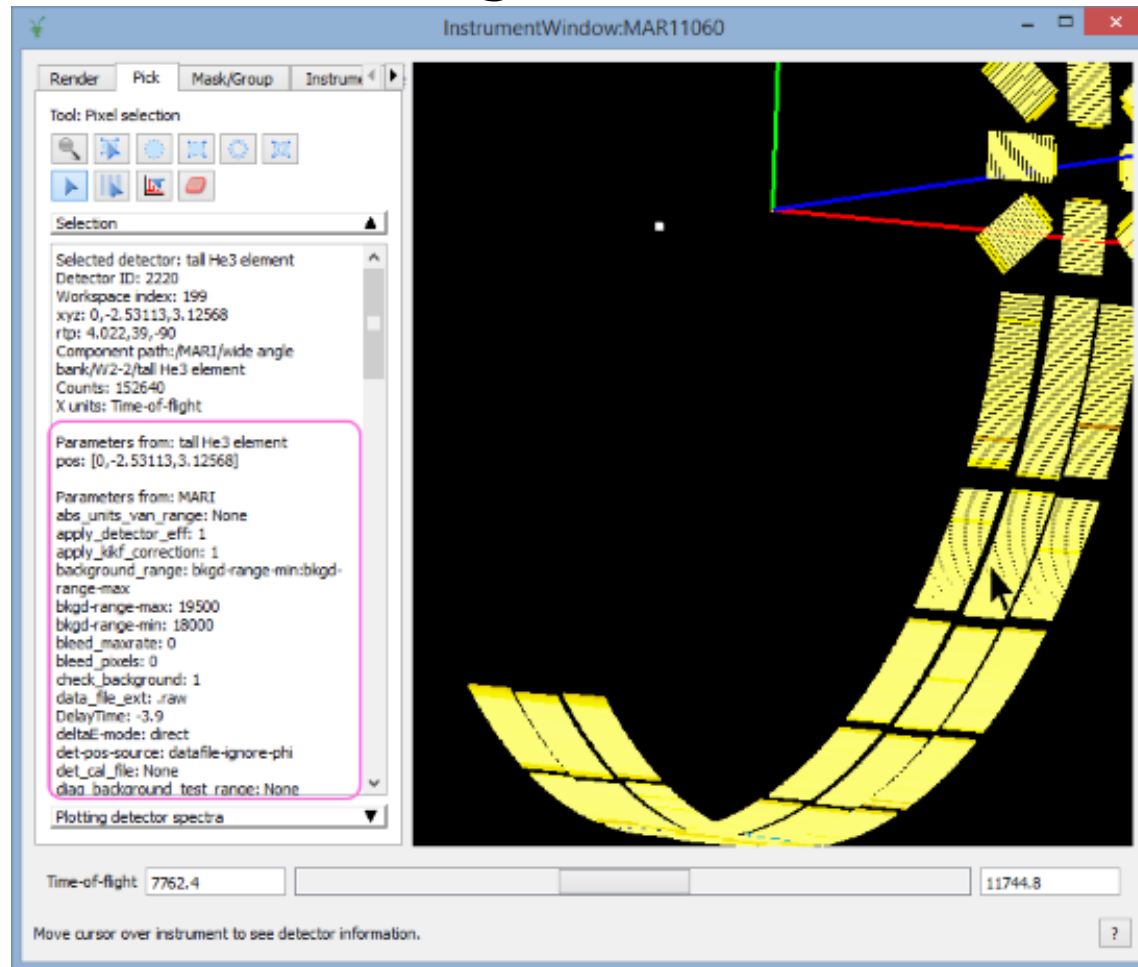
General Plot Options





Instruments

- Instrument parameters are displayed in pick mode
- SaveParameterFile algorithm





Workspace Details

- Workspace details now display origin of instrument

Workspaces

📊 HYS_11388_event

EventWorkspace

Title: tour run

Histograms: 20480

Bins: 1

Histogram

X axis: Time-of-flight / microsecond

Y axis: Counts

Distribution: False

Instrument: HYSPEC (2011-Jul-20 to 2100-Jan-31)

Instrument from: C:\MantidInstall\instrument\HYSPEC_Definition.xml

Parameters from: C:\MantidInstall\instrument\HYSPEC_Parameters.xml

Run start: 2012-Aug-29 13:35:33

Run end: 2012-Aug-29 15:06:26

Events: 361008

Memory used: 69 MB



Multi-Dataset Fitting

- New interface for fitting across multiple data sets
 - Possible before but only from scripts
 - Missing some features of main fitting but is fully usable
- Feedback (as always) is welcome!



Framework



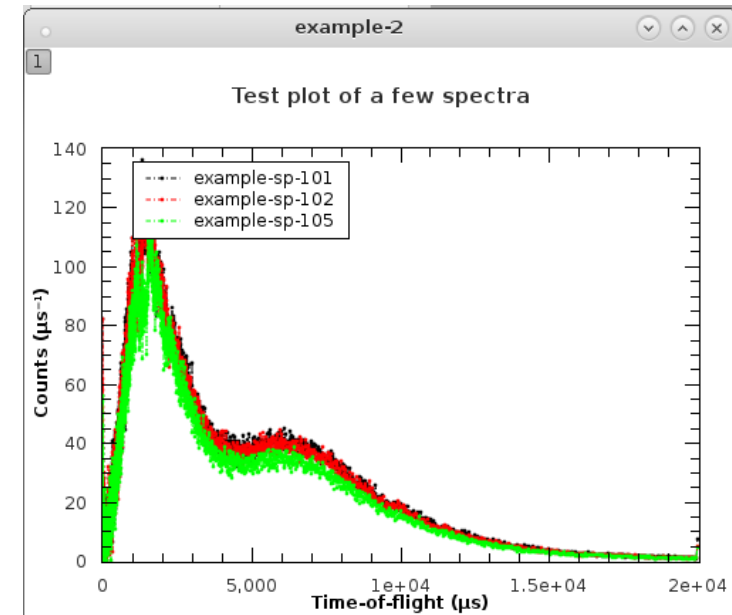
Framework – Improvements

- Instrument definitions
 - 11 updated + new ones: TFXA, IMAT
- Performance: Save/LoadNexusProcessed
 - Speedup for WorkspaceGroups: 138 s => 8 s !
- Algorithms:
 - ~40 new ones
 - ~100 have been improved/extended
- Python command line interface / plotting...



Python Command Line Interface

- Traditional interface: improved error checking
- New module with matplotlib-like interface:
 - Experimental – **feedback!**
 - Interface:
 - Pyplot/matlab, functional
 - Object-oriented
 - *kwargs*: `linestyle='-.', color='red'`
 - Supports:
plotSpectrum / Bin / MD
- Not to be confused:
 - Matplotlib also shipped



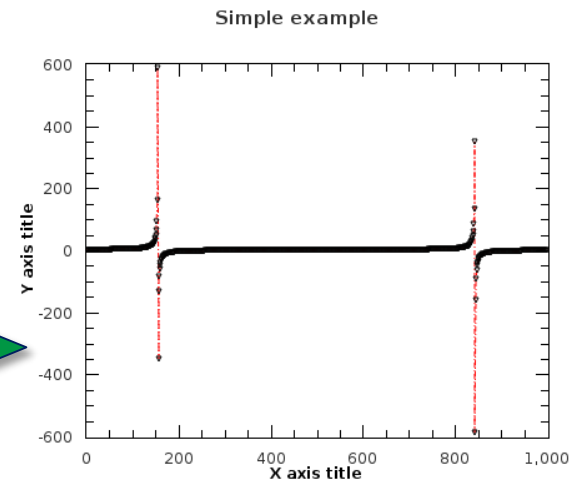
```
In [26]: example = Load("MAR1060.raw", OutputWorkspace="example")
In [27]: lines = plot(example, [100, 101, 104], linestyle='-.')
In [28]: title('Test plot of a few spectra')
```



Python Command Line Interface

- Experimental: `from pymantidplot.future.pyplot import *`
`/ import pymantidplot.future.pyplot as plt`
- Harmonized interface:
 - `plot(source=[{Workspace(s)}], tool={ToolName}, **kwargs)`
 - ToolName: 'plot_spectrum', 'plot_bin', 'plot_md', ...
- Functional interface (pyplot / matlab):

```
from pymantidplot.future.pyplot import *  
import numpy as np  
y = np.tan(np.linspace(-2.28, 2.28, 1000))  
plot(y, linestyle='-.', marker='v', color='red', linewidth=1)  
title('Simple example')  
ylabel('Y axis title')  
xlabel('X axis title')
```



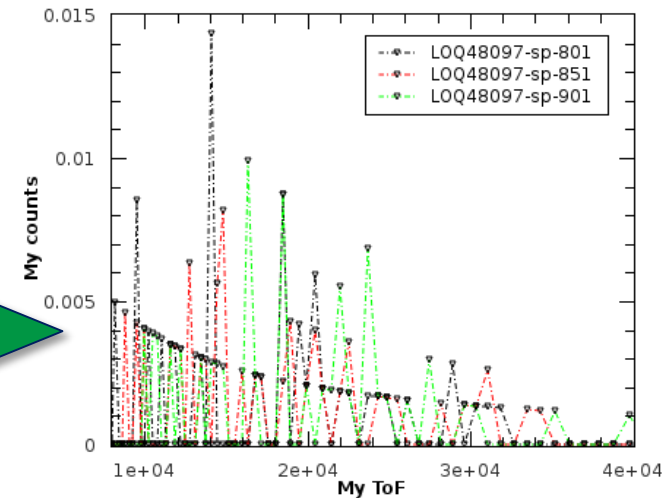


Python Command Line Interface

- Plotting spectra:

```
from pymantidplot.future.pyplot import *  
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(5000, 4e4)  
ylim(0, 0.015)
```

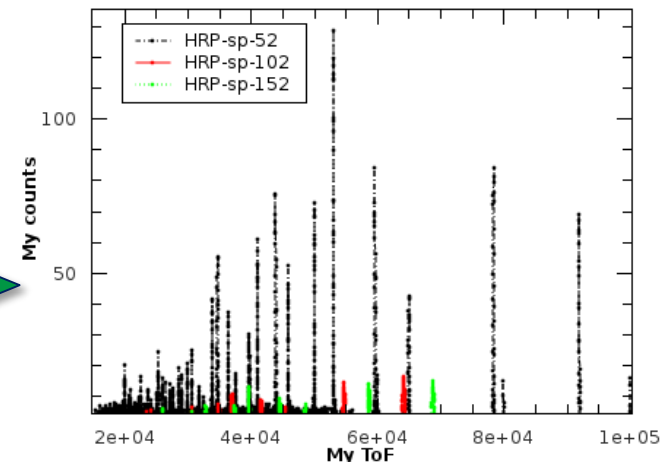
Spectrum plot example



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

```
ws = Load("HRP39182.RAW", OutputWorkspace="HRP")  
lines=plot(ws, 51, 'k-.', ws, 101, 'r', ws, 151, 'g:')  
l0 = lines[0]  
print "X values: ", l0.get_xdata()  
fig = l0.figure()  
fig.suptitle('Spectrum plot example - HRP')  
ax = fig.axes[0][0]  
ax.set_ylabel('My counts')  
ax.set_xlabel('My ToF')  
ax.set_xlim(1.5e4, 1e5)  
ax.set_ylim(5, 135)
```

Spectrum plot example - HRP





Python Command Line Interface

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

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Documentation [edit]

Online Help Pages [\[external\]](#)

Installation [edit]

- System Requirements
- Packages [\[external\]](#), along with installation instructions for supported environments
- Operating system specific issues

Usage [edit]

- Examples of Mantid Usage
- Concepts
- Mantidplot Help
- Algorithm Descriptions [\[external\]](#)
- Fit Functions [\[external\]](#)

Mantid Training Courses [edit]

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

Scripting [edit]

- Python API reference (searchable help) [\[external\]](#)
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- Introduction to NumPy [\[external\]](#)
- Mantid Python without MantidPlot
- Using Mantid with IPython Notebook

Extending Mantid [edit]

- Write your own algorithm
- Create a customized input dialog
- Doxygen code documentation [\[external\]](#)
- Develop
- Algorithms used in testing and validation

Instrument/Technique Specific Mantid Documentation [edit]

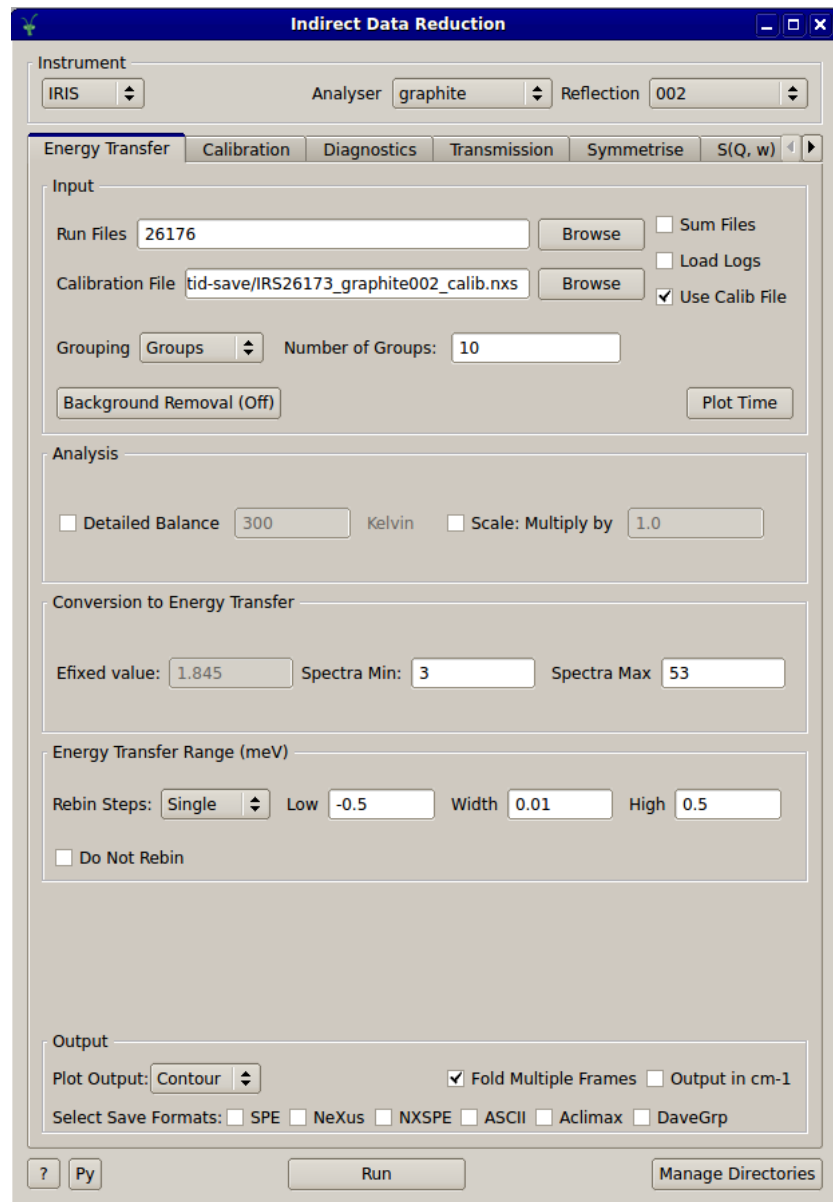
- Scientific Techniques
- VATES



Indirect Inelastic

Updates to Interfaces

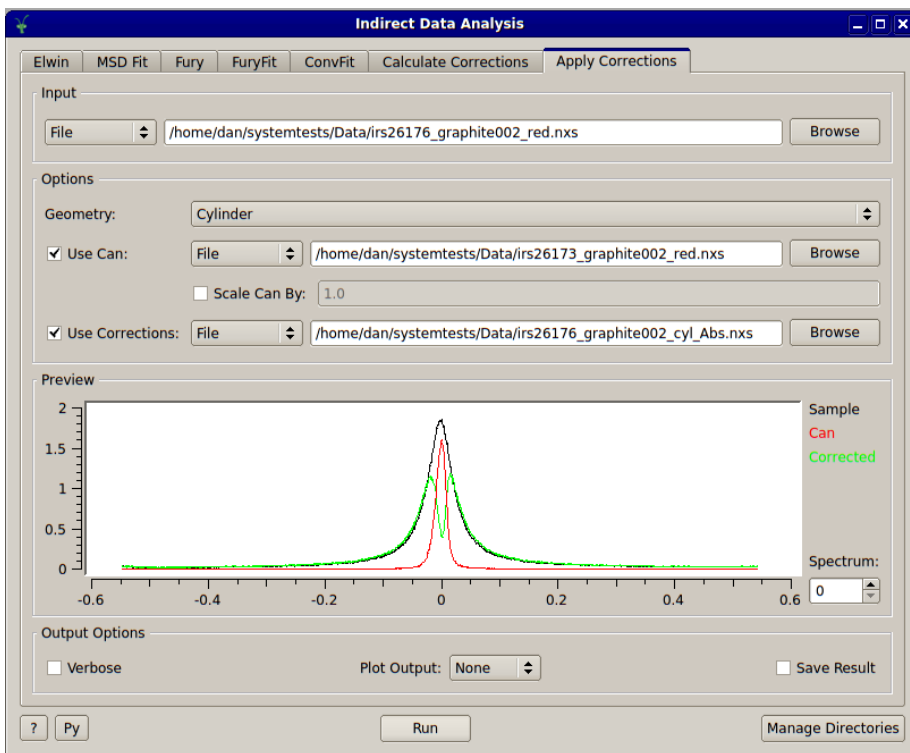
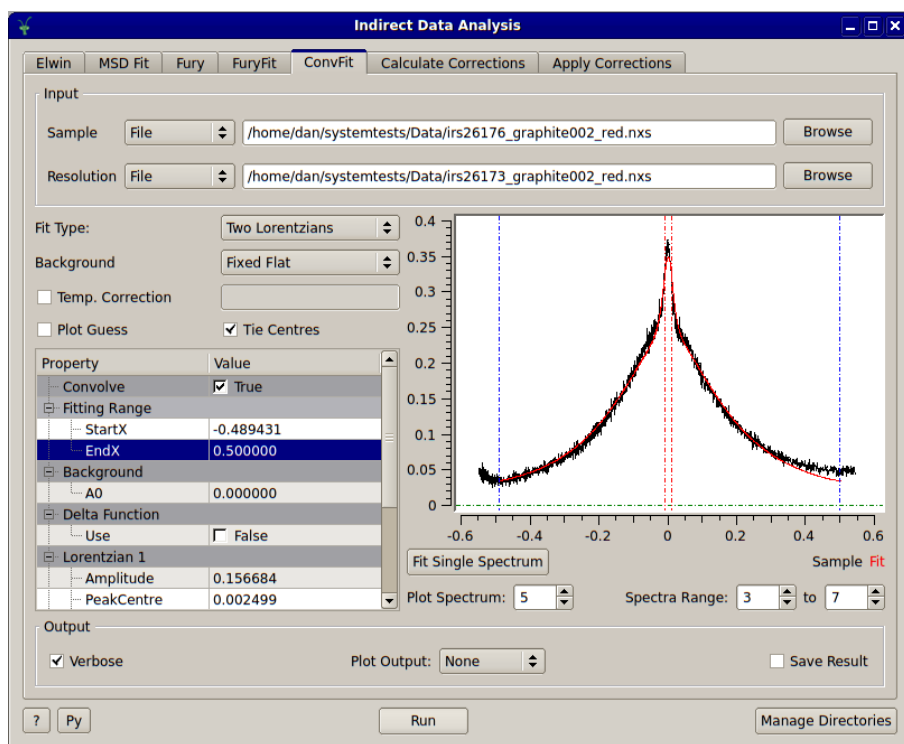
- Name changes
 - **Convert To Energy > Data Reduction**
 - **LoadAscii > Simulation and Tools**



The screenshot shows the 'Indirect Data Reduction' window. At the top, the title bar reads 'Indirect Data Reduction'. Below it, the 'Instrument' section has dropdowns for 'IRIS', 'Analyser' (set to 'graphite'), and 'Reflection' (set to '002'). A tabbed interface follows, with 'Energy Transfer' selected. The 'Input' section contains fields for 'Run Files' (26176), 'Calibration File' (tid-save/IRS26173_graphite002_calib.nxs), and 'Number of Groups' (10). There are checkboxes for 'Sum Files', 'Load Logs', and 'Use Calib File' (checked). A 'Background Removal (Off)' button and a 'Plot Time' button are also present. The 'Analysis' section has checkboxes for 'Detailed Balance' and 'Scale: Multiply by' (1.0). The 'Conversion to Energy Transfer' section includes 'Efired value' (1.845), 'Spectra Min' (3), and 'Spectra Max' (53). The 'Energy Transfer Range (meV)' section has 'Rebin Steps' (Single), 'Low' (-0.5), 'Width' (0.01), 'High' (0.5), and a 'Do Not Rebin' checkbox. The 'Output' section has a 'Plot Output' dropdown (Contour), checkboxes for 'Fold Multiple Frames' (checked) and 'Output in cm-1', and a 'Select Save Formats' section with checkboxes for SPE, NeXus, NXSPE, ASCII, Aclimax, and DaveGrp. At the bottom, there are buttons for '?', 'Py', 'Run', and 'Manage Directories'.

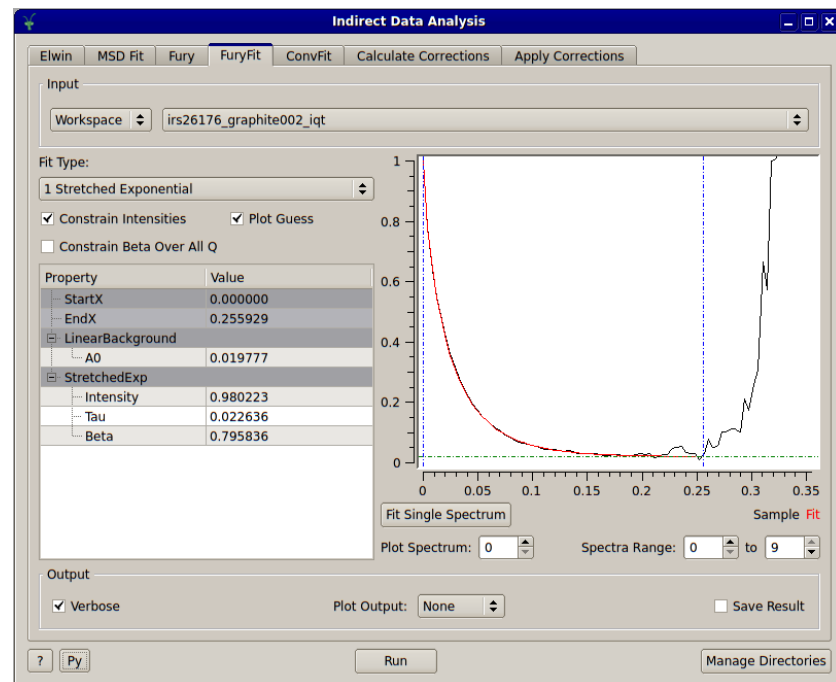
Updates to Interfaces

- Preview plots and spectra selection
- $S(Q, w)$ support on IDR and Bayes



Updates to Interfaces

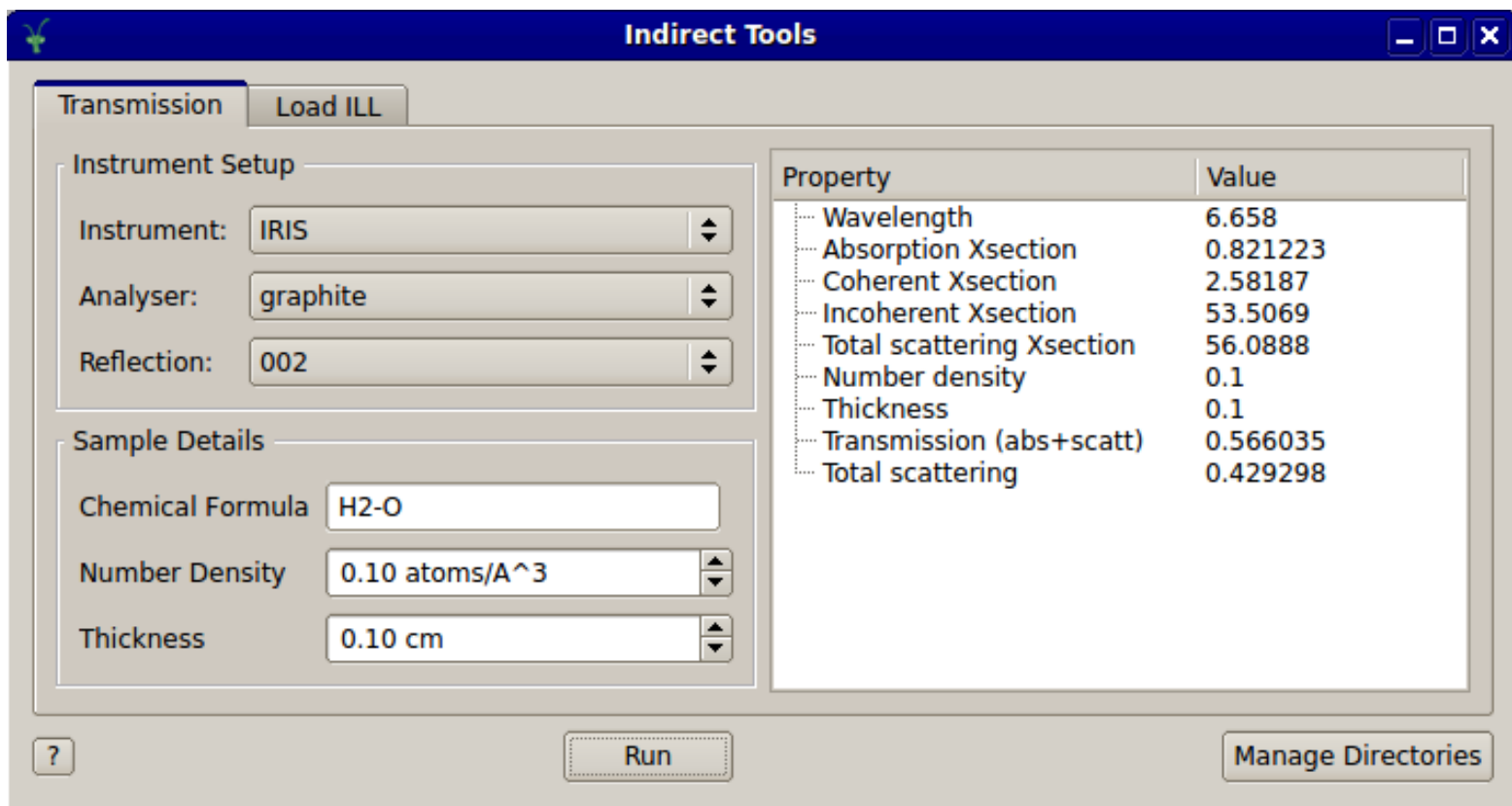
- Python script export for IDR & IDA
 - Modify fitting, reduction, etc. parameters
 - Batch processing



```
MantidPlot: Python Window
File Edit Execute Window
FuryExport.py
1 #####
2 #Python Script Generated by GeneratePythonScript Algorithm
3 #####
4 CropWorkspace(InputWorkspace='irs26176_graphite002_iqt', OutputWorkspace='_furyfit_fit_ws', XMin=0, XMax=0.35)
5 ConvertToHistogram(InputWorkspace='_furyfit_fit_ws', OutputWorkspace='_furyfit_fit_ws', Version=1)
6 ConvertSpectrumAxis(InputWorkspace='_furyfit_fit_ws', OutputWorkspace='_furyfit_fit_ws', Target='ElasticQ',
7 Fit(Function='name=LinearBackground,A0=0.025565,A1=0,ties=(A1=0);name=UserFunction,Formula=Intensity*exp(-
8 GroupWorkspaces(InputWorkspaces='_furyfit_fit_ws_0_Workspace,_furyfit_fit_ws_1_Workspace,_furyfit_fit_ws_2_Workspace,
9 RenameWorkspace(InputWorkspace='_furyfit_fit_ws_9_Workspace', OutputWorkspace='irs26176_graphite002_fury_1S_s0_to_9_9_
10 CopyLogs(InputWorkspace='irs26176_graphite002_iqt', OutputWorkspace='irs26176_graphite002_fury_1S_s0_to_9_9_
11 AddSampleLog(Workspace='irs26176_graphite002_fury_1S_s0_to_9_9_Workspace', LogName='fit_type', LogText='1
12 AddSampleLog(Workspace='irs26176_graphite002_fury_1S_s0_to_9_9_Workspace', LogName='intensities_constrained', LogText='0.980223
13 AddSampleLog(Workspace='irs26176_graphite002_fury_1S_s0_to_9_9_Workspace', LogName='beta_constrained', LogText='0.795836
14 AddSampleLog(Workspace='irs26176_graphite002_fury_1S_s0_to_9_9_Workspace', LogName='end_x', LogText='0.255929
15 AddSampleLog(Workspace='irs26176_graphite002_fury_1S_s0_to_9_9_Workspace', LogName='start_x', LogText='0.000000
16
```

New Interfaces

- Tools, currently contains Transmission calculator and LoadILL
 - Sample transmission calculator (IRIS, OSIRIS, BASIS & VISION)



The screenshot shows the 'Indirect Tools' window with the 'Transmission' tab selected. The interface is divided into three main sections: 'Instrument Setup', 'Sample Details', and a results table.

Instrument Setup

- Instrument: IRIS
- Analyser: graphite
- Reflection: 002

Sample Details

- Chemical Formula: H2-O
- Number Density: 0.10 atoms/A³
- Thickness: 0.10 cm

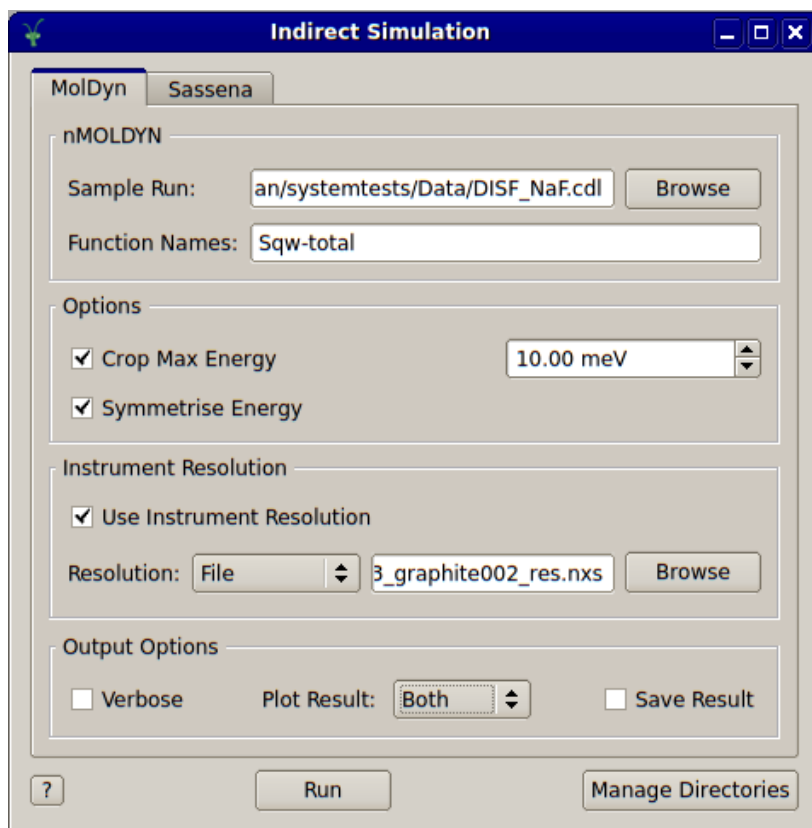
Results Table

Property	Value
Wavelength	6.658
Absorption Xsection	0.821223
Coherent Xsection	2.58187
Incoherent Xsection	53.5069
Total scattering Xsection	56.0888
Number density	0.1
Thickness	0.1
Transmission (abs+scatt)	0.566035
Total scattering	0.429298

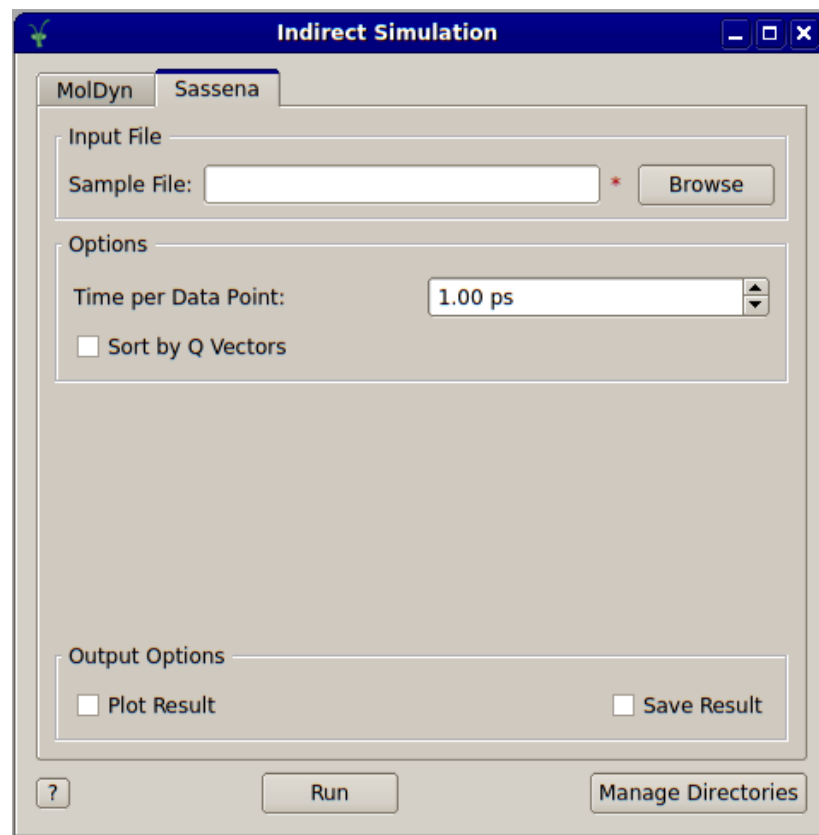
Buttons at the bottom: ? (help), Run, and Manage Directories.

New Interfaces

- Simulation, currently contains loaders for nMOLDYN and Sassena data



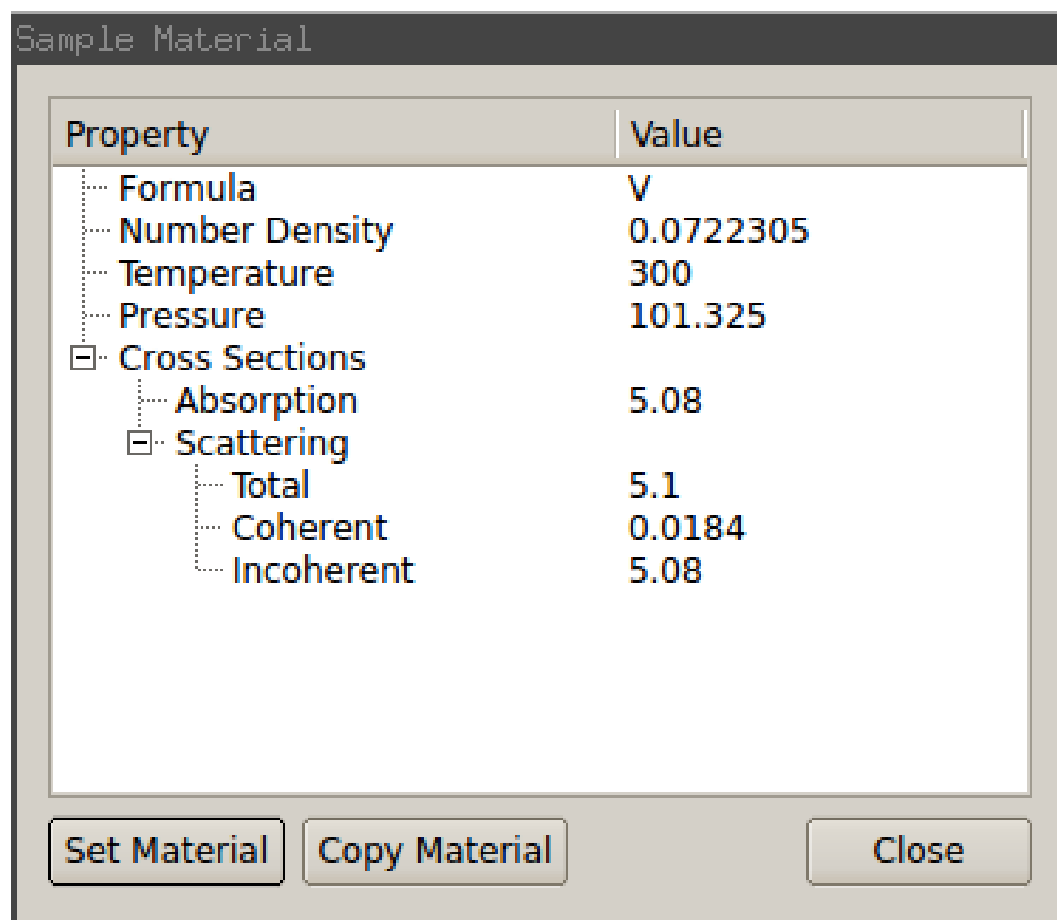
The screenshot shows the 'Indirect Simulation' window with the 'nMOLDYN' tab selected. The 'Sample Run' field contains 'an/systemtests/Data/DISF_NaF.cdl' and the 'Function Names' field contains 'Sqw-total'. Under 'Options', 'Crop Max Energy' is checked with a value of '10.00 meV', and 'Symmetrise Energy' is also checked. Under 'Instrument Resolution', 'Use Instrument Resolution' is checked, and the 'Resolution' is set to 'File' with '3_graphite002_res.nxs' selected. Under 'Output Options', 'Verbose' is unchecked, 'Plot Result' is set to 'Both', and 'Save Result' is unchecked. At the bottom are buttons for '?', 'Run', and 'Manage Directories'.



The screenshot shows the 'Indirect Simulation' window with the 'Sassena' tab selected. The 'Input File' section has an empty 'Sample File' field. Under 'Options', 'Time per Data Point' is set to '1.00 ps' and 'Sort by Q Vectors' is unchecked. Under 'Output Options', both 'Plot Result' and 'Save Result' are unchecked. At the bottom are buttons for '?', 'Run', and 'Manage Directories'.

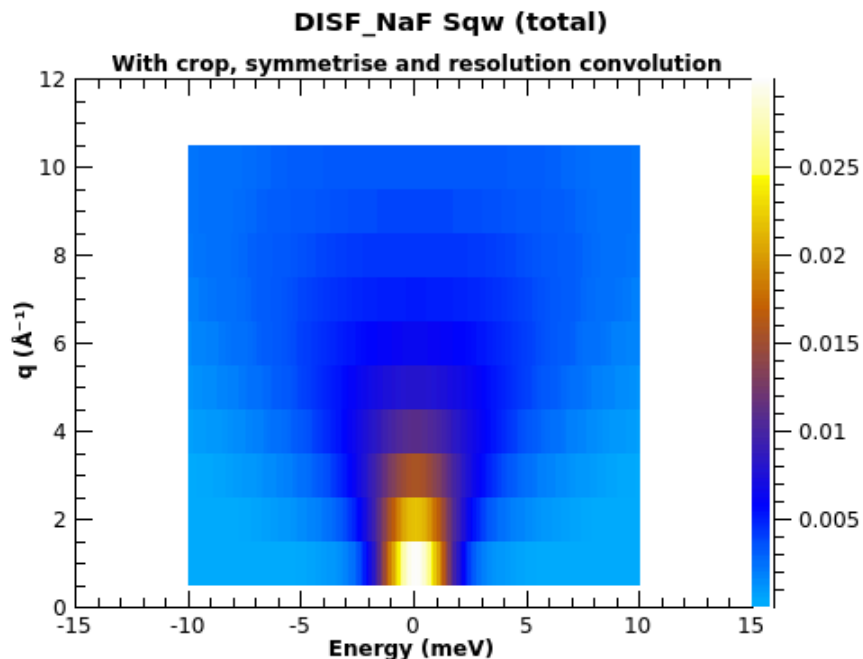
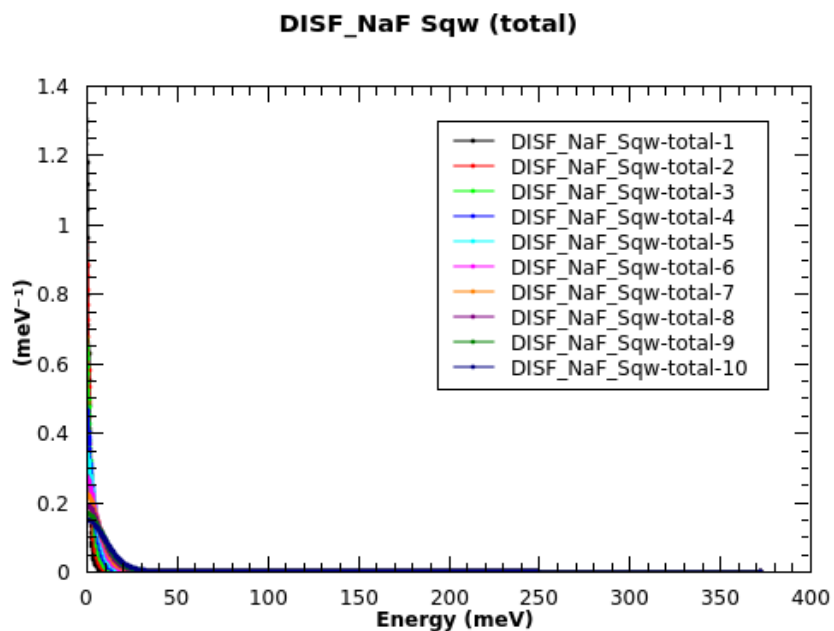
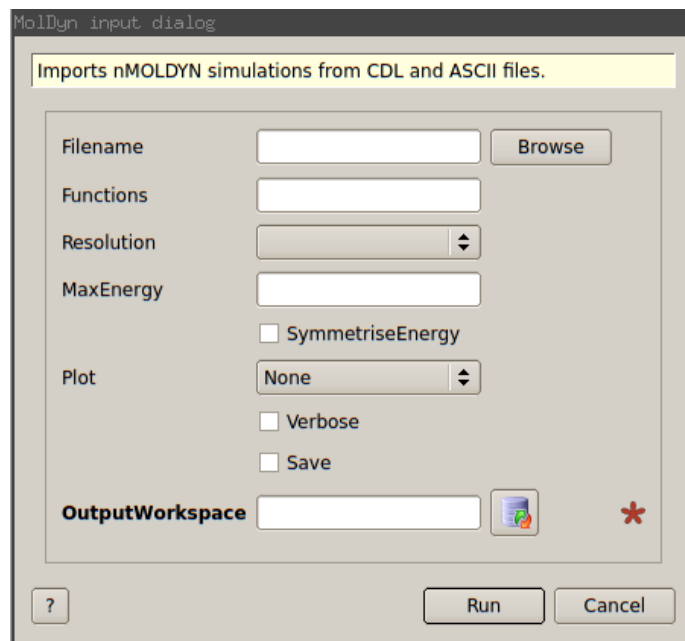
New Interfaces

- Sample material UI
 - Show properties of sample material for a given workspace



Simulation

- New algorithm and updated UI for nMOLDYN
 - Energy crop and symmetrise
 - Convolve $S(q, w)$ with instrument resolution



Simulation

- Scattering cross section scaling in DensityOfStates

DensityOfStates input dialog

Calculates phonon densities of states, Raman and IR spectrum.

File

Function

PeakWidth

SpectrumType

Scale

BinWidth

Temperature

ZeroThreshold

Ions

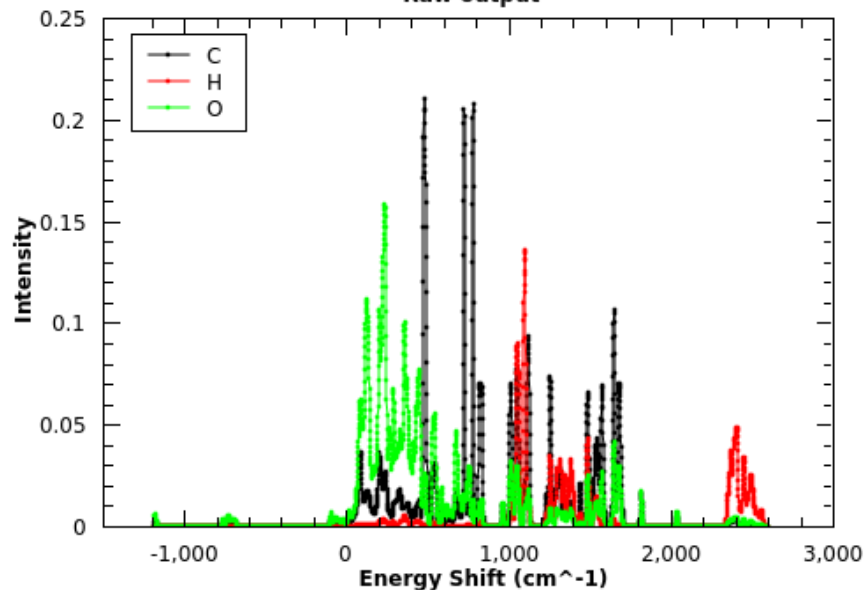
☐ SumContributions

ScaleByCrossSection

OutputWorkspace

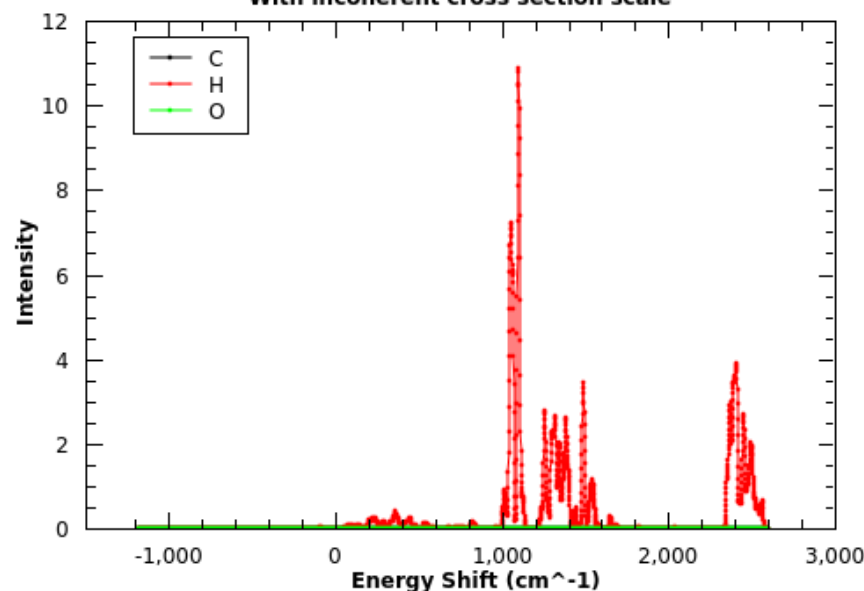
Vibrational densities of states of croconic acid crystal

Raw output



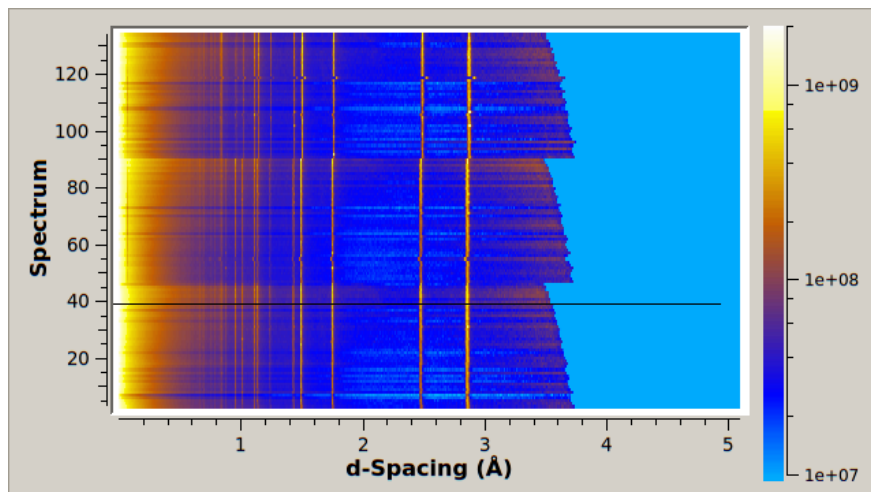
Vibrational densities of states of croconic acid crystal

With incoherent cross section scale

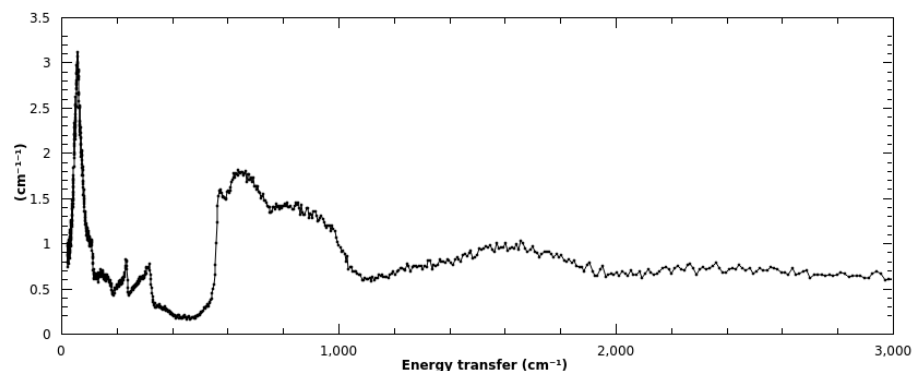


Instrument Support

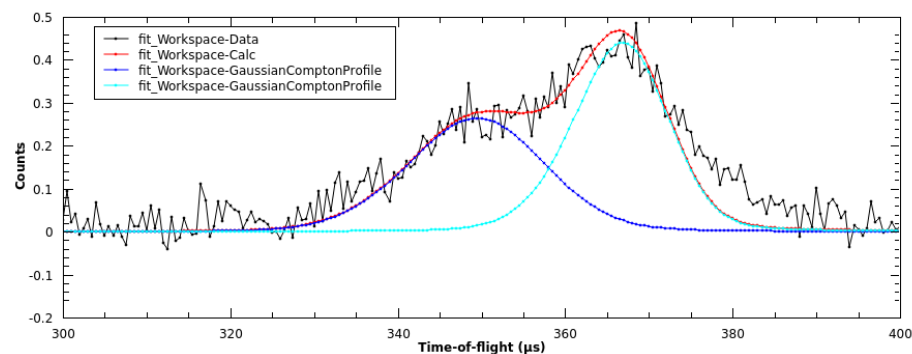
- Support added for TFXA and TOSCA-1 for energy transfer reductions
- Old TFXA data now available on ISIS data archive and ICAT
- Support for VESUVIO close to that of VMS routines



TFX2002: ICE (Ordered)



fit_Workspace

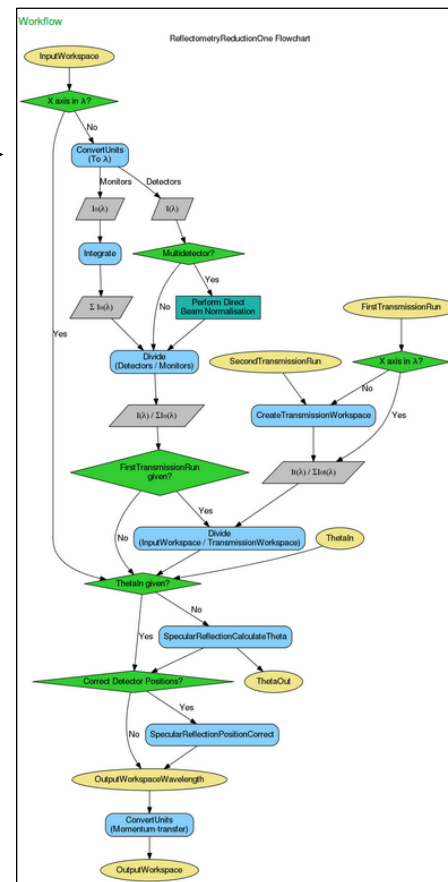




Reflectometry

Algorithms

- LoadNexus & SaveNexus have been optimised
- ReflectometryReductionOne(Auto)
 - Support for workspaces in Wavelength
 - Polarization Correction
 - Workflow diagrams
- CalculateResolution
- SaveRefIThreeColumnAscii





Experimental IPython Notebook Support

IP[y]: Notebook

Processing OFFSPEC Runs Last Checkpoint: Jan 12 09:46 (unsaved changes)

File Edit View Insert Cell Kernel Help

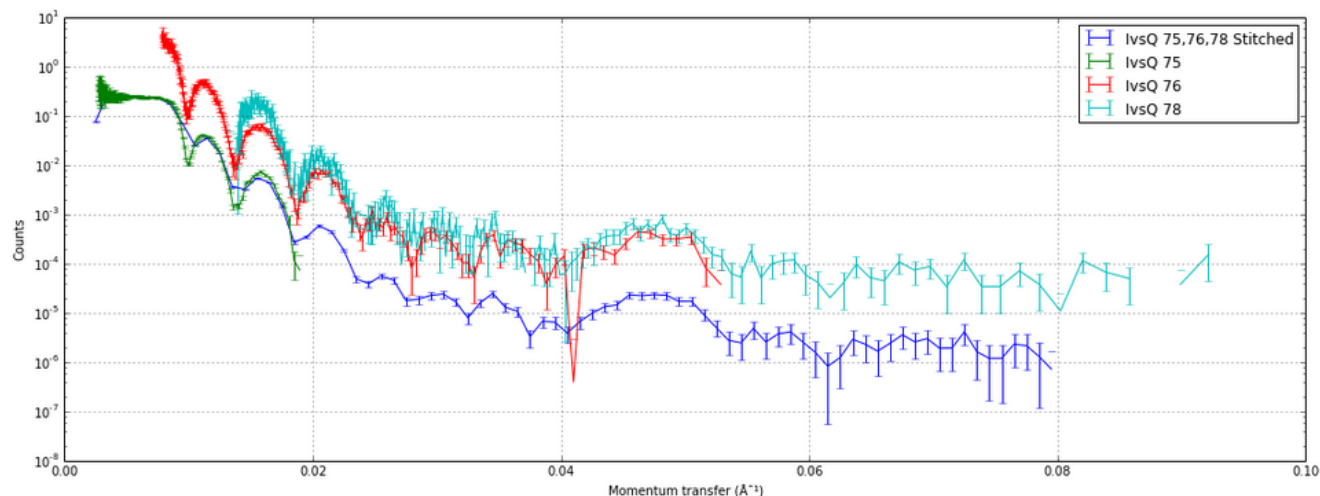
Code Cell Toolbar: None

```
In [3]: #Helper procedure to plot with
def plot_ws(axes, data, label):
    point_data = ConvertToPointData(data)
    axes.errorbar(point_data[0].readX(0), point_data[0].readY(0), yerr=point_data[0].readE(0), label=label)


#Create a figure, 15x5 inches in size, and add a set of axes to it
fig = plt.figure(figsize=(14,5))
axes = fig.add_axes([0,0,1,1])

#Plot the workspaces to the axes
plot_ws(axes, ivq_75_76_78, "IvsQ 75,76,78 Stitched")
plot_ws(axes, ivq_75, "IvsQ 75")
plot_ws(axes, ivq_76, "IvsQ 76")
plot_ws(axes, ivq_78, "IvsQ 78")

#Set some properties of the axes
axes.legend()
axes.grid()
axes.set_xlabel(u"Momentum transfer ( $\text{\AA}^{-1}$ ")
axes.set_ylabel("Counts")
axes.set_yscale("log")
```



Experimental IPython Notebook Support



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- Concepts
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- Algorithms used in testing and validation

Instrument/Technique Specific Mantid Documentation [edit]

- Scientific Techniques
- VATES

Using Mantid with IPython Notebook



Experimental IPython Notebook Support

Download Mantid

Latest release (3.3)

View changes made in [this release](#). It is recommended to use [apt-get](#) or [yum](#) to install Mantid on UNIX.

Installation Instructions: [► OSX](#) [► Red Hat](#) [► Ubuntu](#) [► Windows](#)

[Download source code](#)

Alternative downloads:

[► OSX \(10.8+\)](#) [► Red Hat](#) [► Ubuntu 14.04](#) [► Windows 7/8](#)

[Previous releases](#)

Paraview 3.98.1

Paraview is required to use VATES features.

[Download source code](#)

Alternative downloads:

- [► OSX \(10.8+\)](#)
- [► OSX \(<10.8\)](#)
- [► Ubuntu](#)
- [► Windows XP](#)
- [► Windows 7/8](#)

Sample datasets

Sample datasets for use in Mantid:

- [► Usage Examples](#)
- [► ISIS](#)
- [► ORNL](#)
- [► Muon](#)
- [► Training](#)

Additional examples

Help documentation and examples can be found [here](#)

The IPython notebook is not officially supported for use with Mantid, but an example notebook is provided below.

[► IPython Notebook Example](#)

Nightly build – 2015-01-19

*Nightly development build – minimally tested and **not** recommended for general use.*

[Download source code](#)

View changes in this build in the [recent news](#).

Alternative downloads:

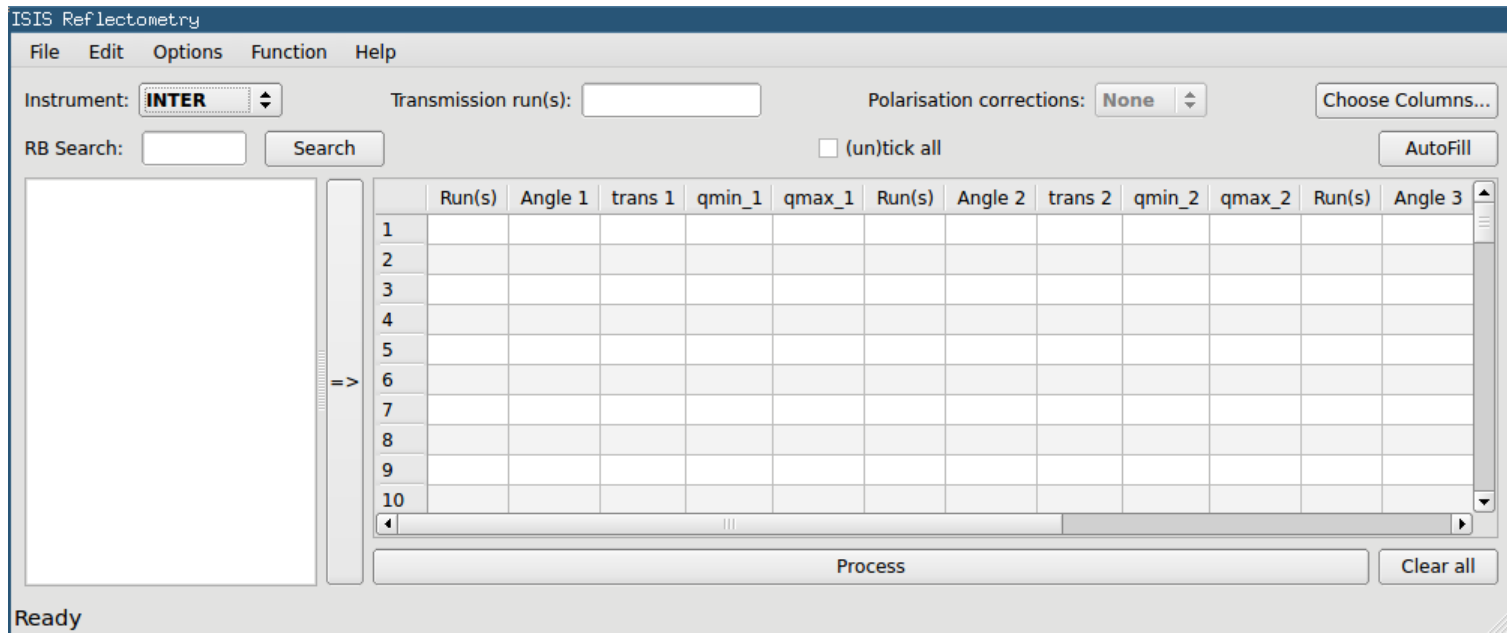
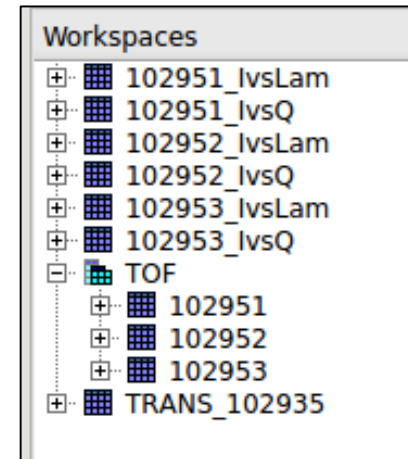
- [► OSX \(10.8+\)](#)
- [► Red Hat](#)
- [► Ubuntu 14.04](#)
- [► Windows 7/8](#)

Previous nightly builds can be found [here](#).

IPython Notebook Example

Reflectometry – ISIS Reduction Interface

- POLREF support added
- Plots are re-used
- Time-of-Flight workspaces are kept
- Improved test suite





Reflectometry – New Reduction Interface

Existing UI

ISIS Reflectometry

File Edit Options Function Help

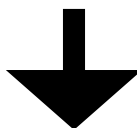
Instrument: **INTER** Transmission run(s): Polarisation corrections: **None** Choose Columns...
RB Search: Search ☐ (un)tick all AutoFill

	Run(s)	Angle 1	trans 1	qmin_1	qmax_1	Run(s)	Angle 2	trans 2	qmin_2	qmax_2	Run(s)	Angle 3	trans 3	qmin_3	qmax_3	dq/q	Scale	Stitch?	Plot?
1	102951	0.25	102935	0.01	0.03	102952	0.65	102935	0.022	0.065	102953	1.5	102935	0.05	0.2	0.01		<input checked="" type="checkbox"/>	Plot
2																		<input type="checkbox"/>	Plot
3																		<input type="checkbox"/>	Plot
4																		<input type="checkbox"/>	Plot

Process Clear all

Ready

New UI



ISIS Reflectometry (Polref)

Reflectometry Edit

Search Runs
Instrument: **INTER**
Investigation Id: Search
Transfer

Process Runs

	Run(s)	Angle	Transmission Run(s)	Q min	Q max	dQ/Q	Scale	Group	Options
1	102951	0.25	102935	0.01	0.03	0.01	1	1	
2	102952	0.65	102935	0.022	0.065	0.01	1	1	
3	102953	1.5	102935	0.05	0.2	0.01	1	1	

0% Instrument: **INTER** Process

Reflectometry – New Reduction Interface

Demo

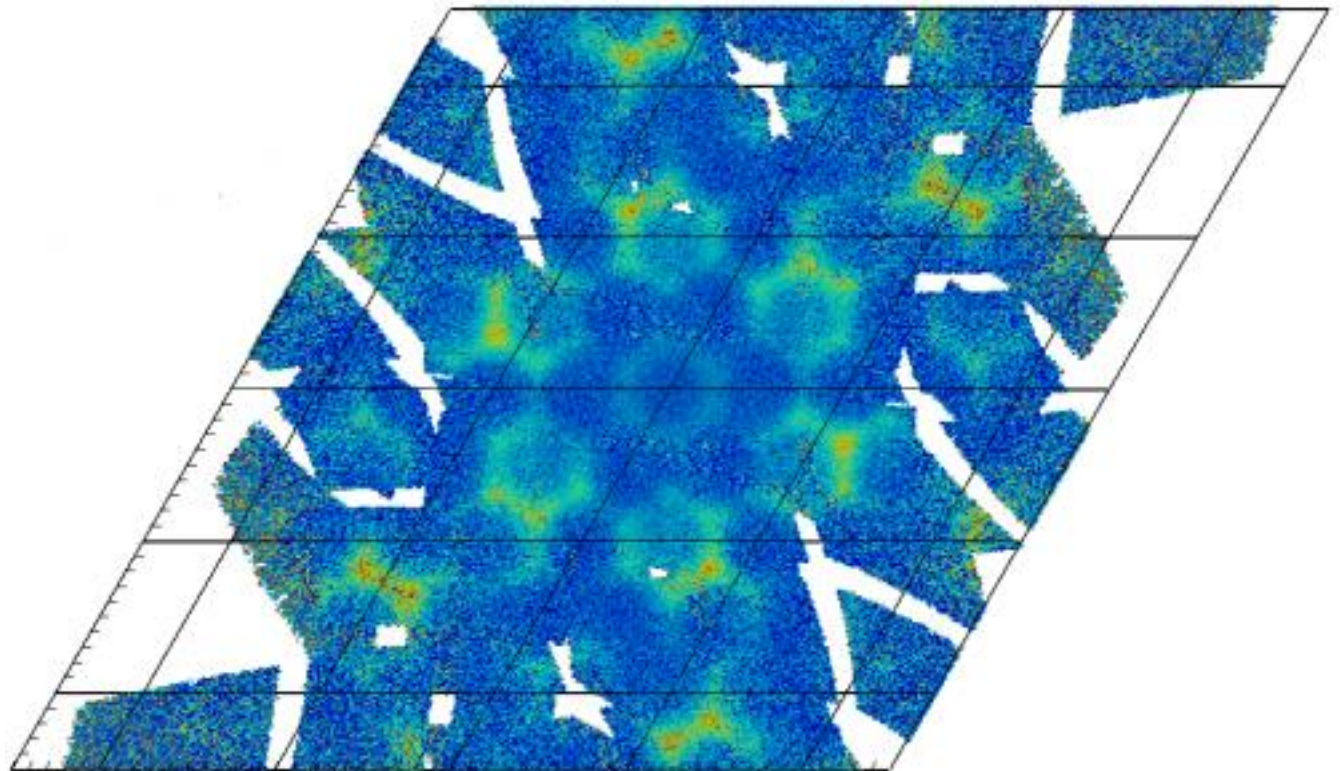


Diffraction



Normalisation

- New Normalisation framework
- Correctly accounts for statistical weights
- **MDNormSCD** for elastic SC diffraction
- Performance enhancements






RebinByTimeAtSample

- New Algorithm **RebinByTimeAtSample**
- Works in the elastic case
- Determines absolute event times at the sample, and rebins to a histogram form.
- Aid and comparison for event filtering by fast logs.
- Shared codebase with **RebinByPulseTime**

Rebins with an x-axis of relative time at sample for comparing event arrival time at the sample environment.

InputWorkspace	<input type="text"/>	*
Params	<input type="text"/>	*
OutputWorkspace	<input type="text"/>	 *



Point Groups

- Point groups and symmetry classes have been added as core concepts in Mantid.
- Minimal usage at the moment in the codebase
- Exposed to python
- Documentation with usage examples available here http://docs.mantidproject.org/nightly/concepts/Point_groups.html
- Contribution to Mantid from the PSI



Symmetry Operations

```
# Symmetry Operations

from mantid.geometry import SymmetryOperation, SymmetryOperationFactoryImpl

symOp = SymmetryOperationFactoryImpl.Instance().createSymOp("x,y,-z")

hkl = [1, -1, 3]
hklPrime = symOp.apply(hkl)

print "Mirrored hkl:", hklPrime
```

Output:

```
Mirrored hkl: [1,-1,-3]
```



Point Groups

```
# Point Groups

from mantid.geometry import PointGroup, PointGroupFactoryImpl

pg = PointGroupFactoryImpl.Instance().createPointGroup("m-3m")

hkl1 = [2, 0, 0]
hkl2 = [0, 0, -2]
hkl3 = [0, 1, 2]

print "Are [2,0,0] and [0,0,-2] equivalent?", pg.isEquivalent(hkl1, hkl2)
print "Are [2,0,0] and [0,1,2] equivalent?", pg.isEquivalent(hkl1, hkl3)
```

Output:

```
Are [2,0,0] and [0,0,-2] equivalent? True
Are [2,0,0] and [0,1,2] equivalent? False
```



Symbol	Symmetry operation
x, y, z	Identity
$-x, -y, -z$	Inversion
$-x, -y, z$	2-fold rotation around z
$x, y, -z$	Mirror plane perpendicular to z
$-x, -y, z+1/2$	2_1 screw axis along z

Crystal system	Laue classes
Cubic	$m\bar{3}, m\bar{3}m$
Hexagonal	$6/m, 6/mmm$
Trigonal	$\bar{3}, \bar{3}m$
Tetragonal	$4/m, 4/mmm$
Orthorhombic	mmm
Monoclinic	$2/m$
Triclinic	$\bar{1}$



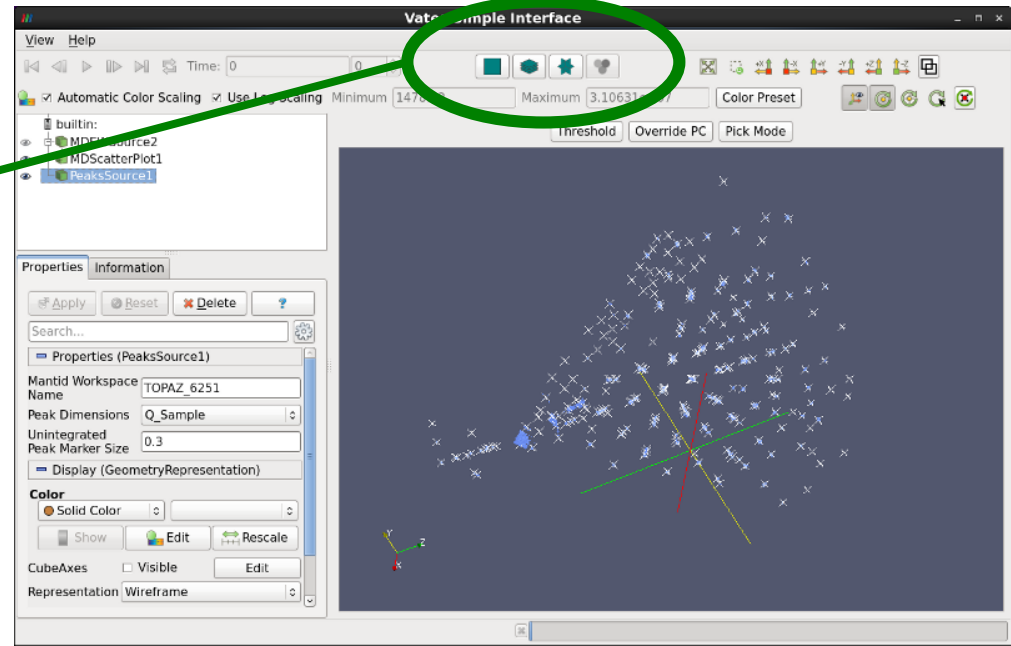
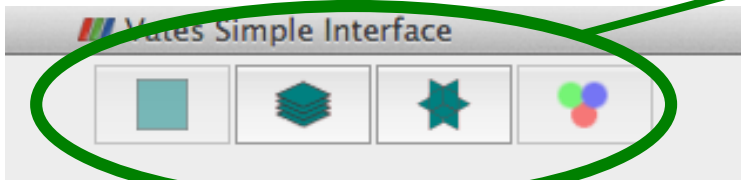
Fixes and Improvements

- **SaveLaueNorm** new peak format
- Connected Component Analysis engine fixed
- Issue with integrated region off detector edge fixed
- OrientedLattices exposes `qFromHKL` and `hklFromQ`
- V3D gives direction angles, also via python
- Several key bugfixes around the VSI particularly view-switching.



Paraview SCD progress

- Technique dependent initial view in VSI
 - http://www.mantidproject.org/VatesSimpleInterface_v2
- Not quite ready for this release
 - More powerful in-situ rebinning
 - Faster representations at lower memory overhead
 - Faster slicing
 - Multi-window mode
 - A less confusing interface





SANS



SANS

http://www.mantidproject.org/ISIS_SANS

• [SANS User Interface](#)

- Compatibility of different web browsers with canSAS XML data file:
[/Rendering_canSAS1D_in_Web_Browsers](#)

For those who really want to know more:

- [Top level view of the what and how of ISIS SANS data reduction](#)

Q-resolution: TOFSANSResolutionByPixel

$$(\sigma_Q)^2 = \frac{4\pi^2}{12\lambda^2} \left[3\left(\frac{R_1}{L_1}\right)^2 + 3\left(\frac{R_2}{L_3}\right)^2 + \left(\frac{\Delta R}{L_2}\right)^2 \right] + Q^2 \left(\frac{\sigma_\lambda}{\lambda}\right)^2$$

where

$$\frac{1}{L_3} = \frac{1}{L_1} + \frac{1}{L_2}$$

$$(\sigma_\lambda)^2 = (\Delta\lambda)^2/12 + (\sigma_{\text{moderator}})^2$$

- R_1 equals SourceApertureRadius
- R_2 equals SampleApertureRadius
- ΔR equals DeltaR
- $\sigma_{\text{moderator}}$ equals SigmaModerator

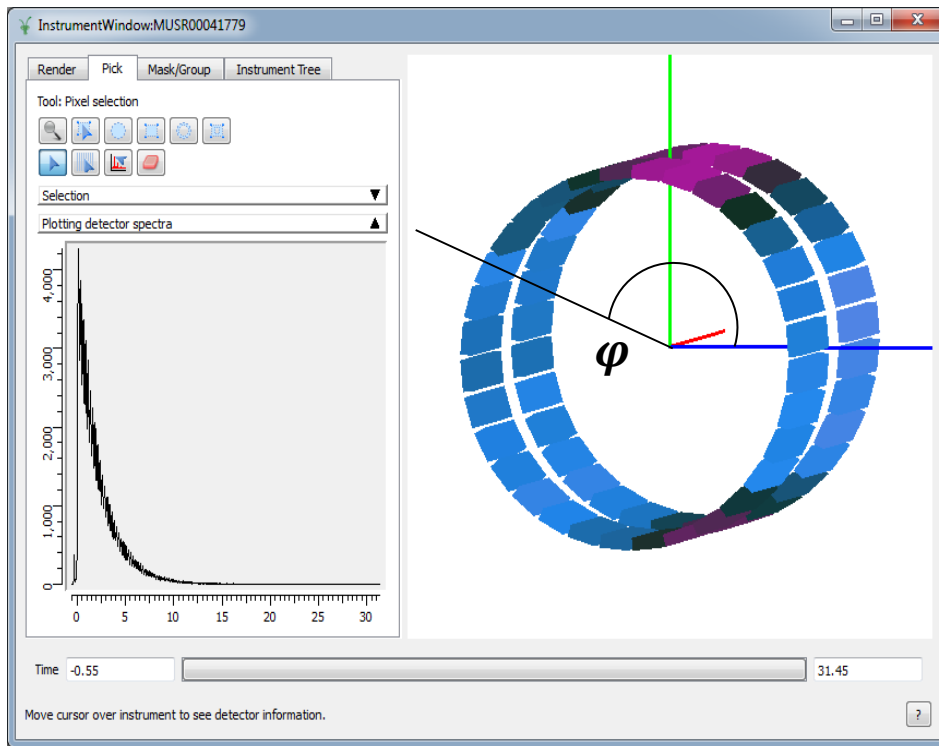


Muon



Muon

- New algorithm: **PhaseQuad**
 - Input workspace



The 'PhaseQuad input dialog' box contains the following fields and controls:

- InputWorkspace:** MUSR00041779 (highlighted with a green box)
- OutputWorkspace:** MUSR00041779_out
- PhaseTable:** (dropdown menu, highlighted with a blue box)
- PulseOver:** 60
- MeanLag:** 127.702
- DoublePulse:** ☐
- PhaseList:** s/muon/HISSDATA64.INF (highlighted with a blue box) with a 'Browse' button.

Buttons at the bottom: Run, Cancel.

- Input phase table/list

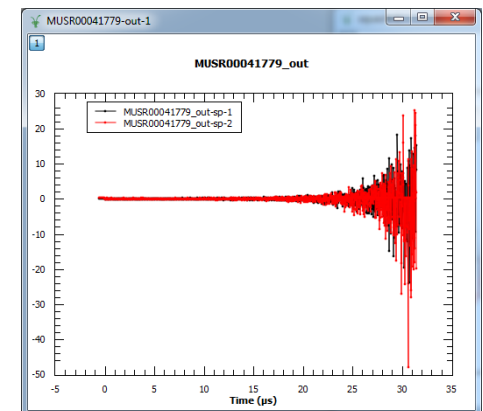
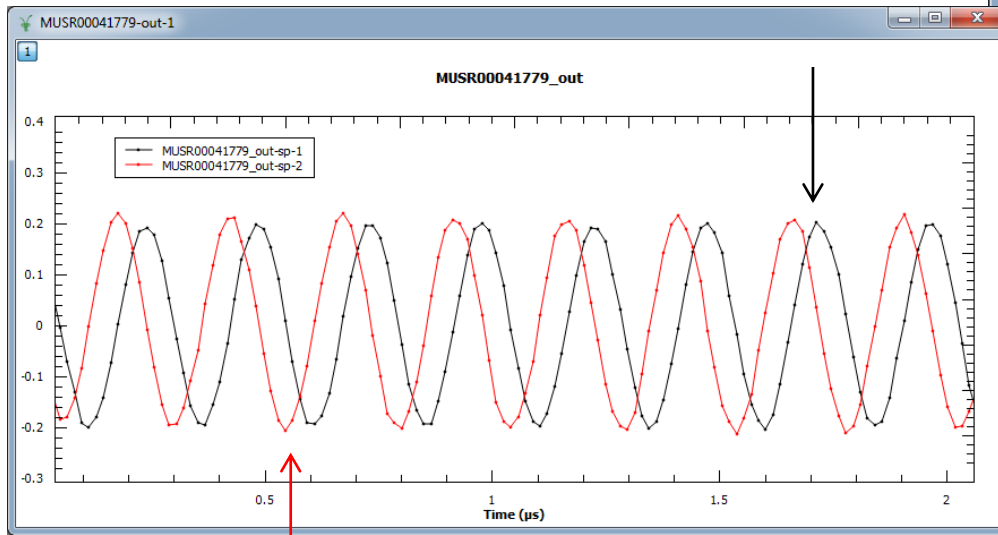
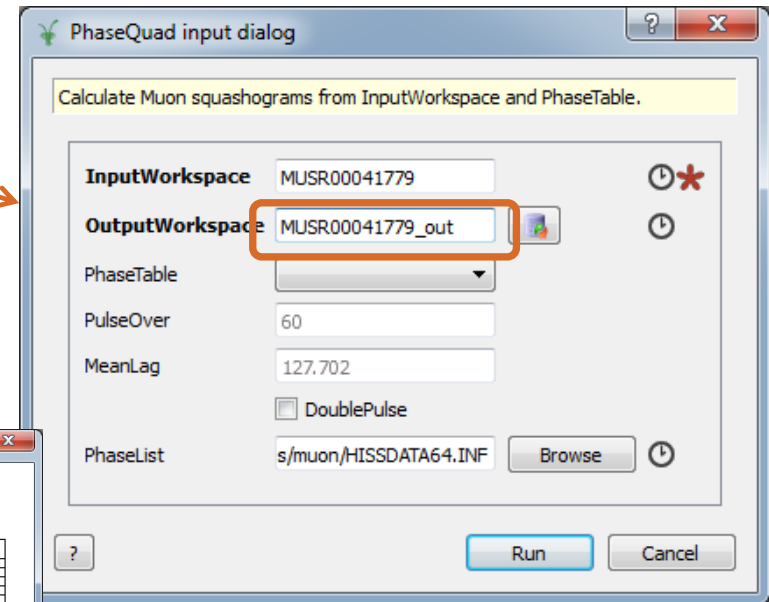
The table window 'Table-1 - phase_table' displays the following data:

	detOK[Y]	efficiency[Y]	phase[Y]	deadtime[Y]
0	true	52.2763	5.27893	-2.23607
1	true	54.4907	5.04726	-2.23607
2	true	56.5433	4.79076	-2.23607
3	true	59.4986	4.7026	-2.23607
4	true	59.8075	4.39657	-2.23607
5	true	63.3368	4.19069	-2.23607
6	true	59.9464	4.16979	-2.23607
7	true	55.0105	3.99395	-2.23607
8	true	53.5545	3.75544	-2.23607
9	true	56.6145	3.5111	-2.23607



Muon

- New algorithm: **PhaseQuad**
 - Output workspace:
 - 2 spectra
 - **Real** + Imaginary
 - Lab-frame





Autoreduction



What is it?

- A system for running user provided* reduction scripts as soon as data becomes available from the beamline.
- Can work with Mantid.
- A web application to manage and monitor automatic reduction jobs.

The screenshot shows the ISIS Auto-reduction web application. At the top, there is a header with the Science & Technology Facilities Council logo, a welcome message for Marcus, and navigation links for All Jobs, Job Queue, Admin, and Logout. The main title is "ISIS Auto-reduction". Below this is a search bar and two tabs: "View By Experiment Number" (selected) and "View By Job Number". The main content area displays a table of reduction jobs. The table has columns for experiment names (MERLIN, TEST, WISH, LET), job status (Completed), and last updated time. Each experiment name has a corresponding "Edit Reduction Variables" link. The WISH experiment is expanded, showing a list of job numbers (28912, 28906, 28903, 28905, 28904) and their status.

Experiment	Status	Last updated
MERLIN		
TEST		
WISH		
28912	Completed	Jan. 9, 2015, 4:59 p.m.
28906	Completed	Jan. 8, 2015, 2:09 p.m.
28903	Completed	Jan. 8, 2015, 2:07 p.m.
28905	Completed	Jan. 8, 2015, 2:07 p.m.
28904	Completed	Jan. 8, 2015, 2:07 p.m.
LET		

If you require any help with this website please visit the [Help Pages](#) or [Contact Us](#).



Features


- Automatically run user provided scripts as early as possible.
- Provide different scripts for different runs / experiments.
- Modify script variables through the web interface.

The screenshot shows the 'ISIS Auto-reduction' web interface. At the top, there is a header with the Science & Technology Facilities Council logo, a welcome message 'Welcome, Marcus', and navigation links for 'All Jobs', 'Job Queue', 'Admin', and 'Logout'. The main heading is 'ISIS Auto-reduction', followed by 'LET'. A status box indicates 'All reduction jobs complete.' with a link to 'View upcoming saved variable changes'. Below this, there are two tabs: 'By Experiment Reference Number' and 'By Run Number Range'. The 'By Run Number Range' tab is active, showing fields for 'Run Number Start' (1), 'Finished (Optional)', 'energy_bins' (-1, 0.002, 0.95), 'wb_run' (LET00005545.raw), 'sample_run' (LET00006278.nxs), and 'incident_energy' (7.0). There is an 'Advanced Variables' section with a right-pointing arrow. On the right side, there is an 'Additional Actions' box with links for 'Preview Reduction Script' and 'Reset to default values'. At the bottom, there are 'Cancel' and 'Submit Changes' buttons. A footer note states: 'If you require any help with this website please visit the [Help Pages](#) or [Contact Us](#).'



Features

- See an overview of reduction jobs from the web application.

 Science & Technology
Facilities Council

Welcome, Marcus [All Jobs](#) [Job Queue](#) [Admin](#) [Logout](#)

ISIS Auto-reduction

[View By Experiment Number](#) [View By Job Number](#)


>	MERLIN	Edit Reduction Variables
>	TEST	Edit Reduction Variables
✓	WISH	
	28912	Completed Last updated: Jan. 9, 2015, 4:59 p.m.
	28906	Completed Last updated: Jan. 8, 2015, 2:09 p.m.
	28903	Completed Last updated: Jan. 8, 2015, 2:07 p.m.
	28905	Completed Last updated: Jan. 8, 2015, 2:07 p.m.
	28904	Completed Last updated: Jan. 8, 2015, 2:07 p.m.
>	LET	Edit Reduction Variables

If you require any help with this website please visit the [Help Pages](#) or [Contact Us](#).



Features

- View details of each run.

Welcome, Marcus [All Jobs](#) [Job Queue](#) [Admin](#) [Logout](#)

ISIS Auto-reduction

Reduction Job #28905

Status: Completed Instrument: WISH RB Number: 1410048 Last Updated: Jan. 8, 2015, 2:07 p.m. Data: \\isis\inst\$\\NDXWISH\Instrument\data\CYCLE_14_2\WISH00028905.nxs	Start: Jan. 8, 2015, 2:07 p.m. Finish: Jan. 8, 2015, 2:07 p.m. Duration: 23 seconds Reduced: \\isis\inst\$\\NDXWISH\Instrument\data\cycle_14_2\auto-reduced\1410048\28905\
---	--

[➤ Re-run reduction job](#)

If you require any help with this website please visit the [Help Pages](#) or [Contact Us](#).



Features

- Re-run reduction jobs with new script variables (or a new script).

The screenshot displays the 'ISIS Auto-reduction' web interface. At the top, there is a navigation bar with the Science & Technology Facilities Council logo, a welcome message 'Welcome, Marcus', and links for 'All Jobs', 'Job Queue', 'Admin', and 'Logout'. The main heading is 'ISIS Auto-reduction', followed by 'Reduction Job #28905'. A summary box contains the following details:

Status: Completed	Start: Jan. 8, 2015, 2:07 p.m.
Instrument: WISH	Finish: Jan. 8, 2015, 2:07 p.m.
RB Number: 1410048	Duration: 23 seconds
Last Updated: Jan. 8, 2015, 2:07 p.m.	
Data: \\isis\inst\$NDXWISH\instrument\data\CYCLE_14_2\WISH00028905.nxs	
Reduced: \\isis\inst\$NDXWISH\instrument\data\cycle_14_2\auto-reduced\1410048\28905\	

Below the summary box is a section titled 'Re-run reduction job'. It contains a 'Re-run description' field, and three rows of input fields for 'Minimum Extents' (value: -3,-5,-4,-5.0), 'Psi Increments' (value: 2, 0.5), and 'Maximum Extents' (value: 5,2,4,30.0). An 'Advanced Variables' section is collapsed, showing a 'Number of Runs to Merge' field with the value 5. To the right of these fields is a box titled 'Additional Actions' with three links: 'Preview Reduction Script', 'Reset to default values', and 'Reset to current script and values'. At the bottom of the form are two buttons: 'Cancel' and 'Re-run with new variables'. The footer of the page includes the text 'If you require any help with this website please visit the [Help Pages](#) or [Contact Us](#)'.



Features

- Access it from many devices.





Demo

(Hopefully)



Contact

Marcus Noble

marcus.noble@stfc.ac.uk

Lottie Greenwood

lottie.greenwood@stfc.ac.uk

System Problems / Help

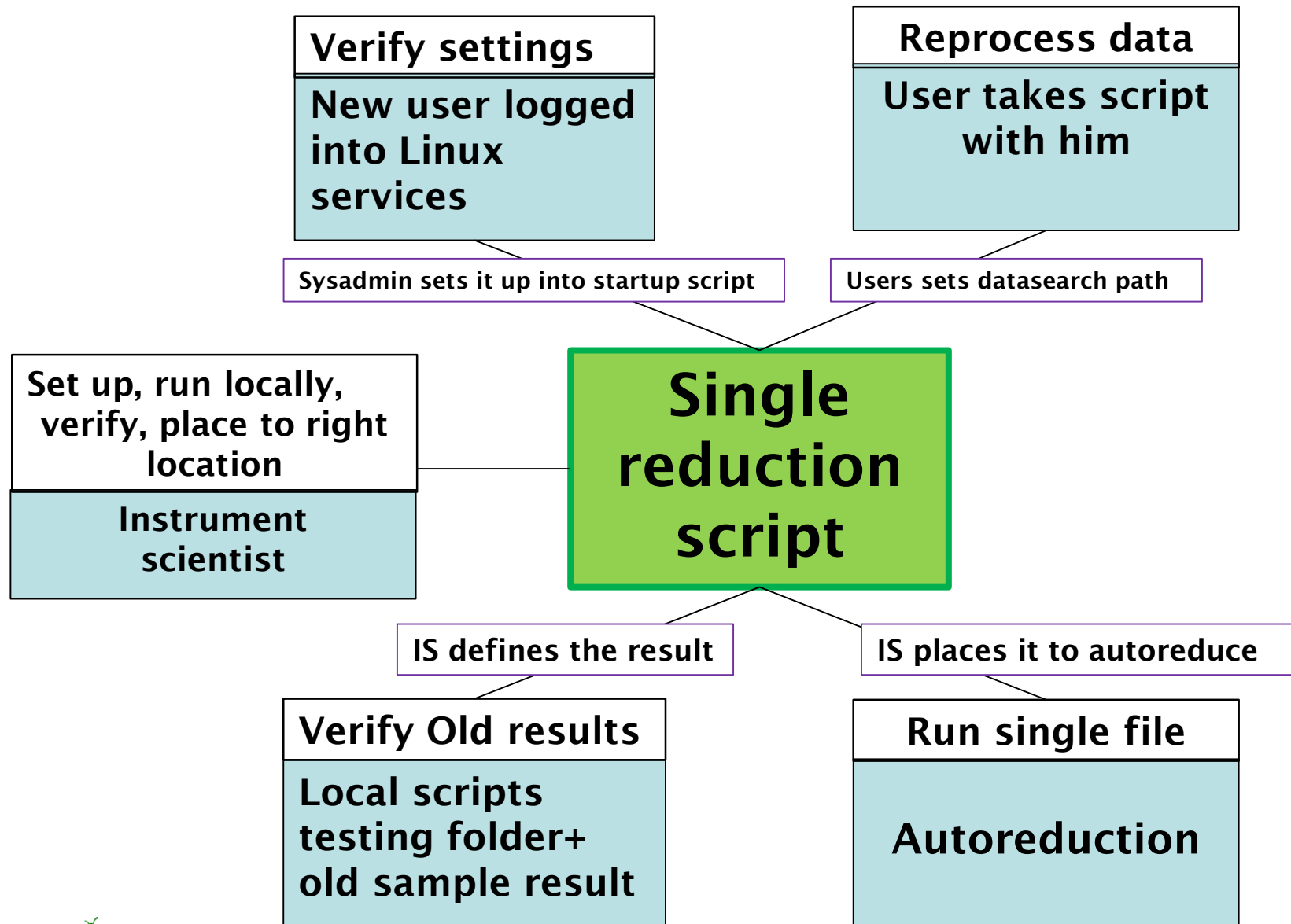
isisdata@stfc.ac.uk




Direct Inelastic



Direct Inelastic Single reduction script for all instruments and usage





Direct Inelastic: Bugfixes and efficiency improvements

MAIN CHANGES:

- Direct inelastic script properties are fully defined by InstrumentParameters.xml file (you can not add or modify property not defined in this file)
- Works with autoreduction too.
- Correct parameter file while processing old experimental results
- Consistent data loading (Source-file and Source-workspace behave the same way)
- 3-fold increase in unit/system test coverage.
- *Later rebinning and internal multirep mode (in progress)*



Next Release



Release v3.4

- Planned Release Date: Friday 1st May 2015
- Mantid Roadmap
 - <http://trac.mantidproject.org/mantid/roadmap>



Thank you

