MANTID

Mantid Release Presentation

Release 3.3

ISIS

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EUROPEAN SPALLATION SOURCE

Tessella Technology & Consulting

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

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)

100%

Number of tickets: closed: 924 testing: 0 reopened: 0 inprogress: 0 assigned: 0 new: 0 Total: 924

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

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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

redhat ENTERPRISE 6

Windows 7

- Limited support for
  - Windows 8 64 bit
  - Fedora 20
  - RHEL 7 64bit

Windows 8

fedora 20

RED HAT ENTERPRISE LINUX 7

- No Longer supported
  - Ubuntu 12.04 64 bit

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User Interface

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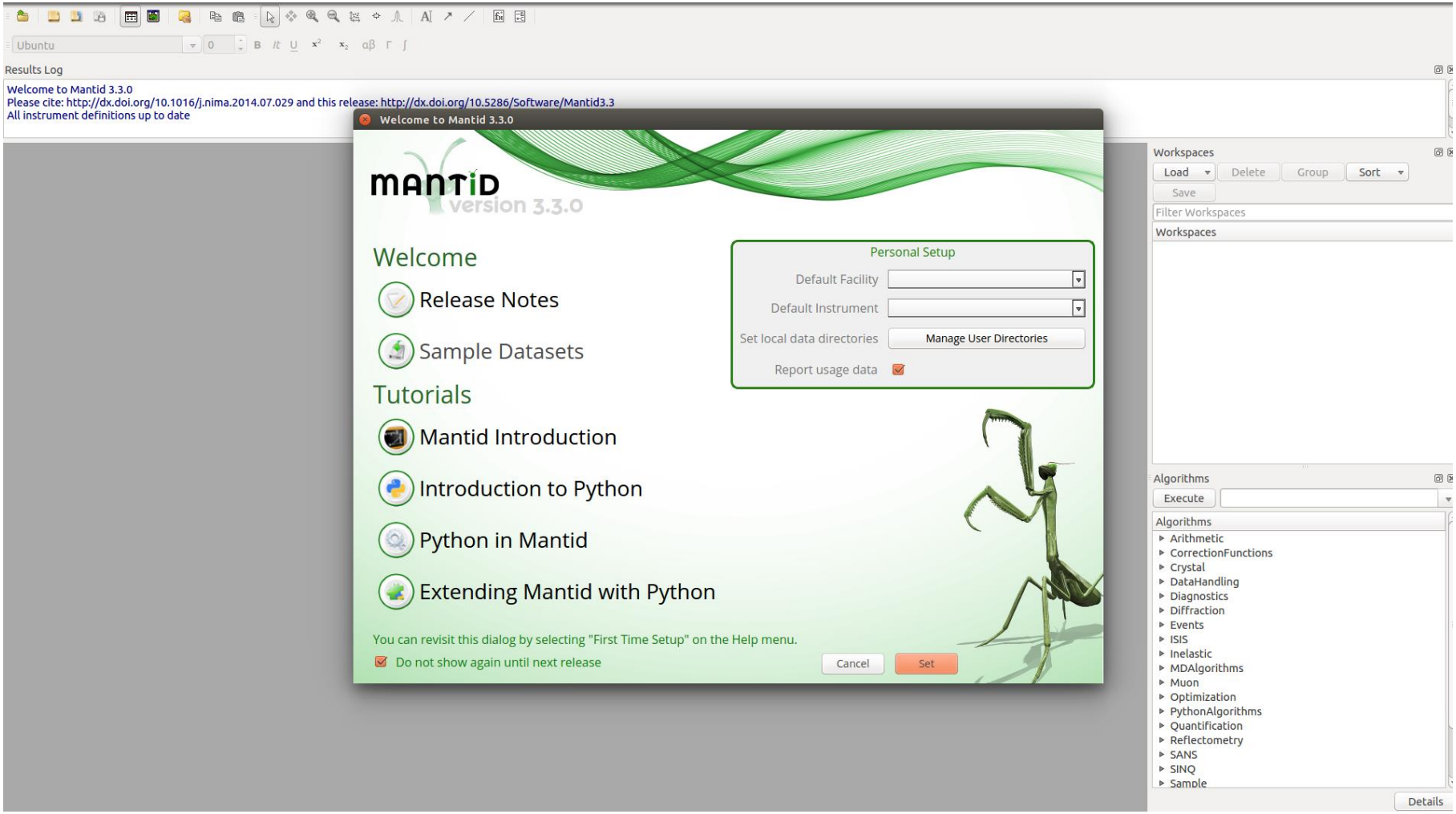
Artwork & Startup

- New artwork provided by ORNL graphics team



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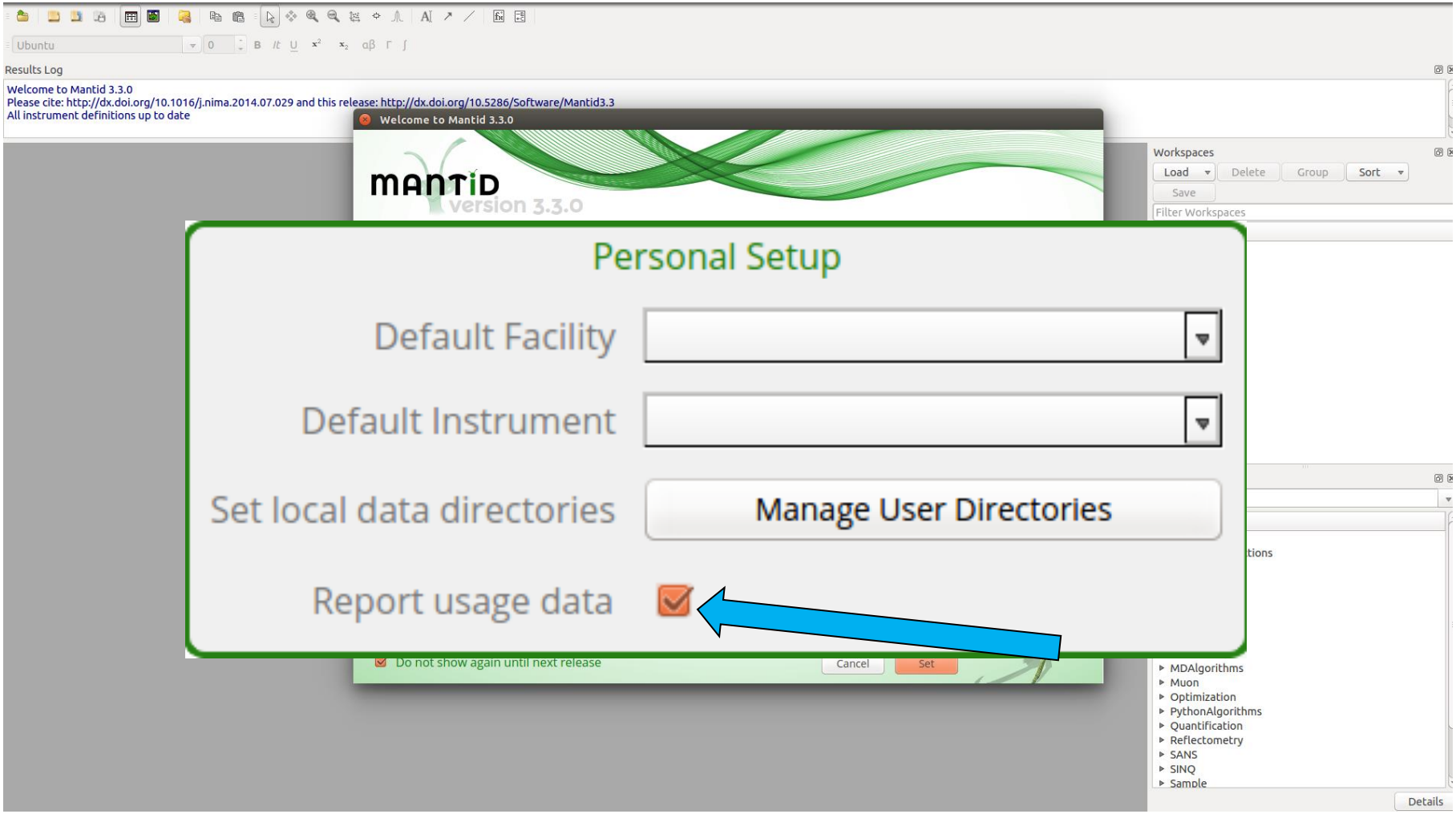

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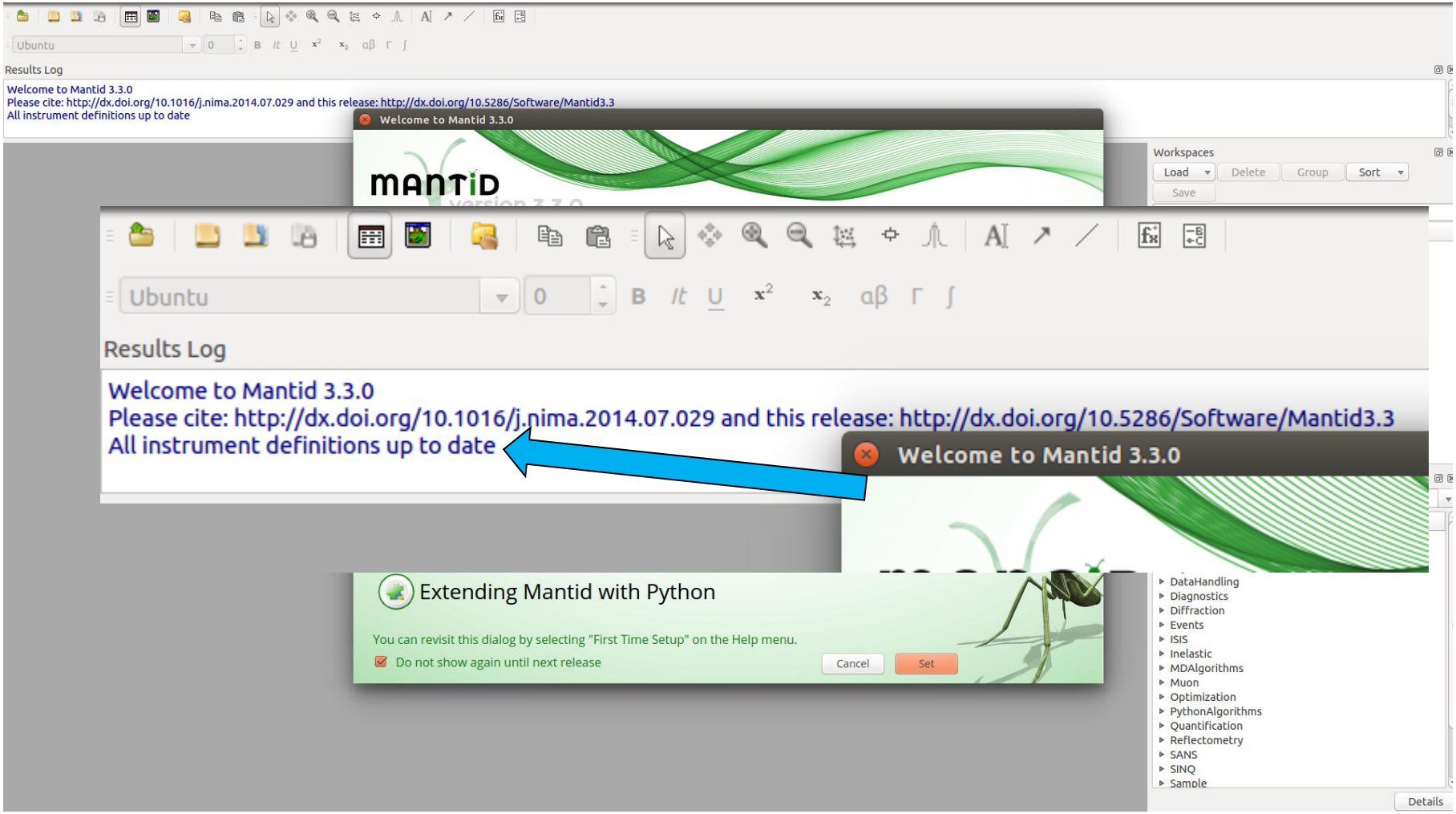
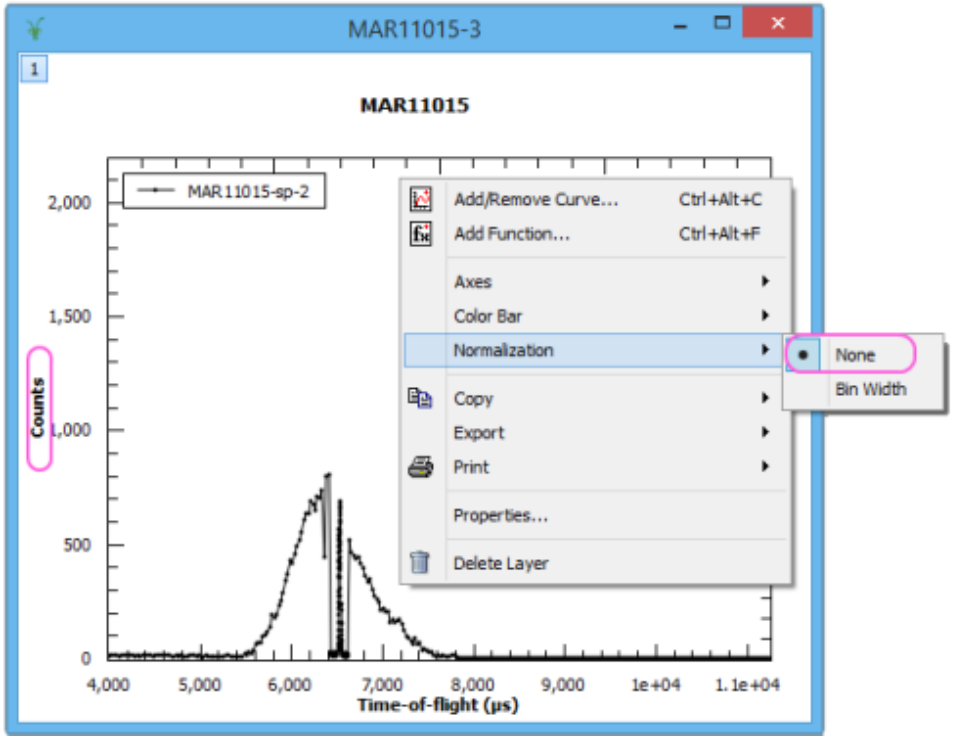
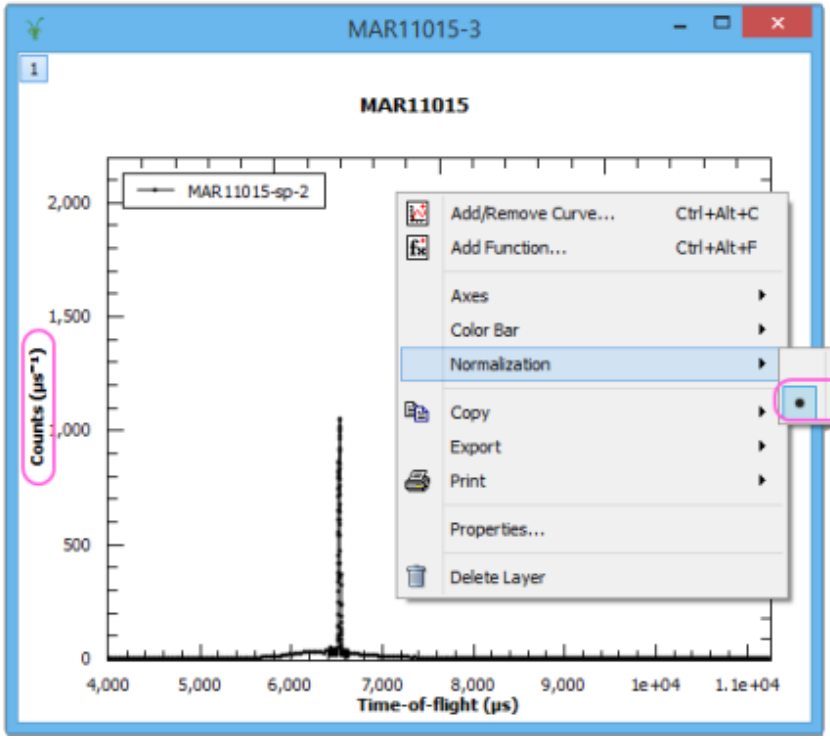


Histogram Plots

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





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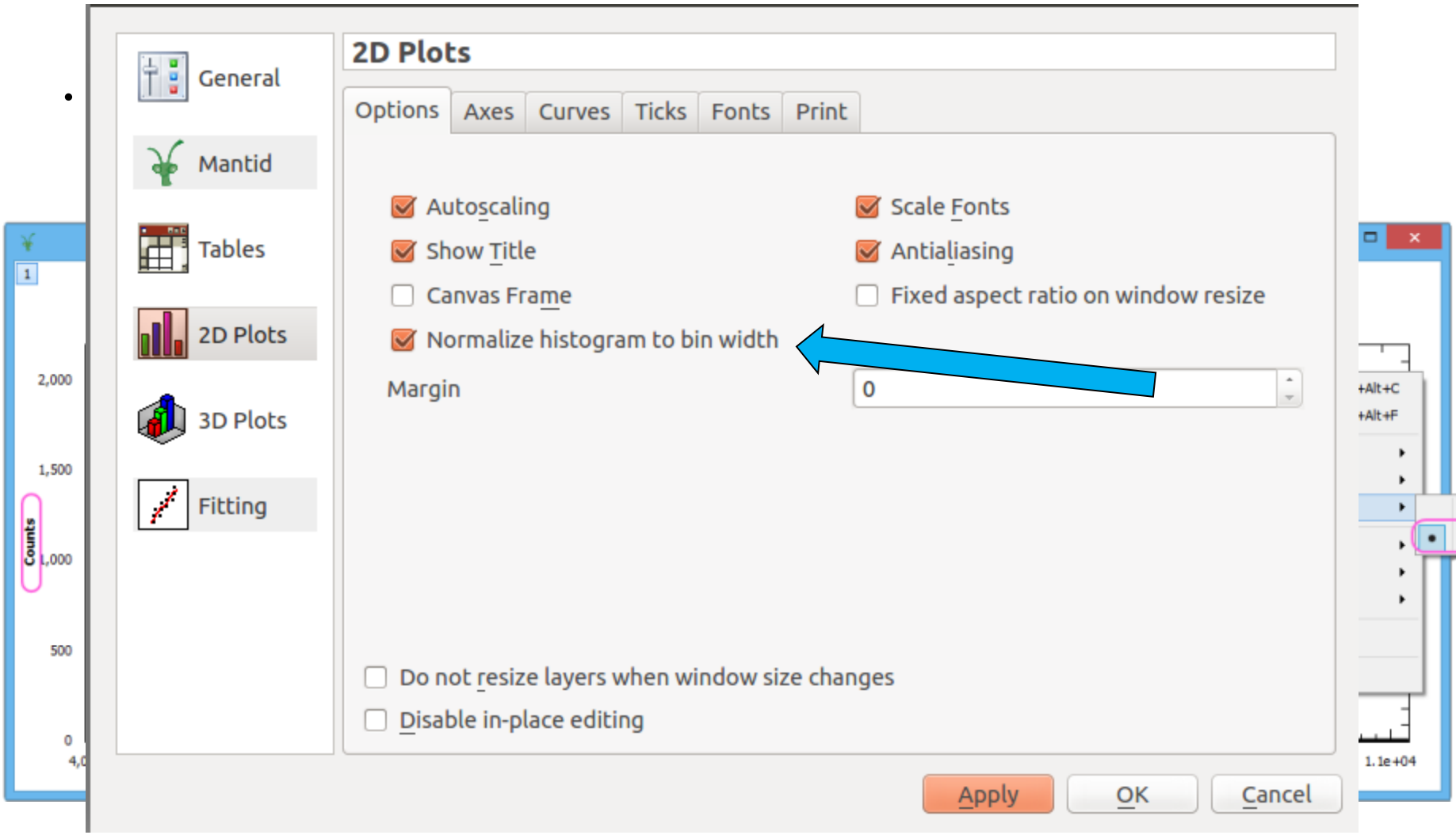
Histogram Plots



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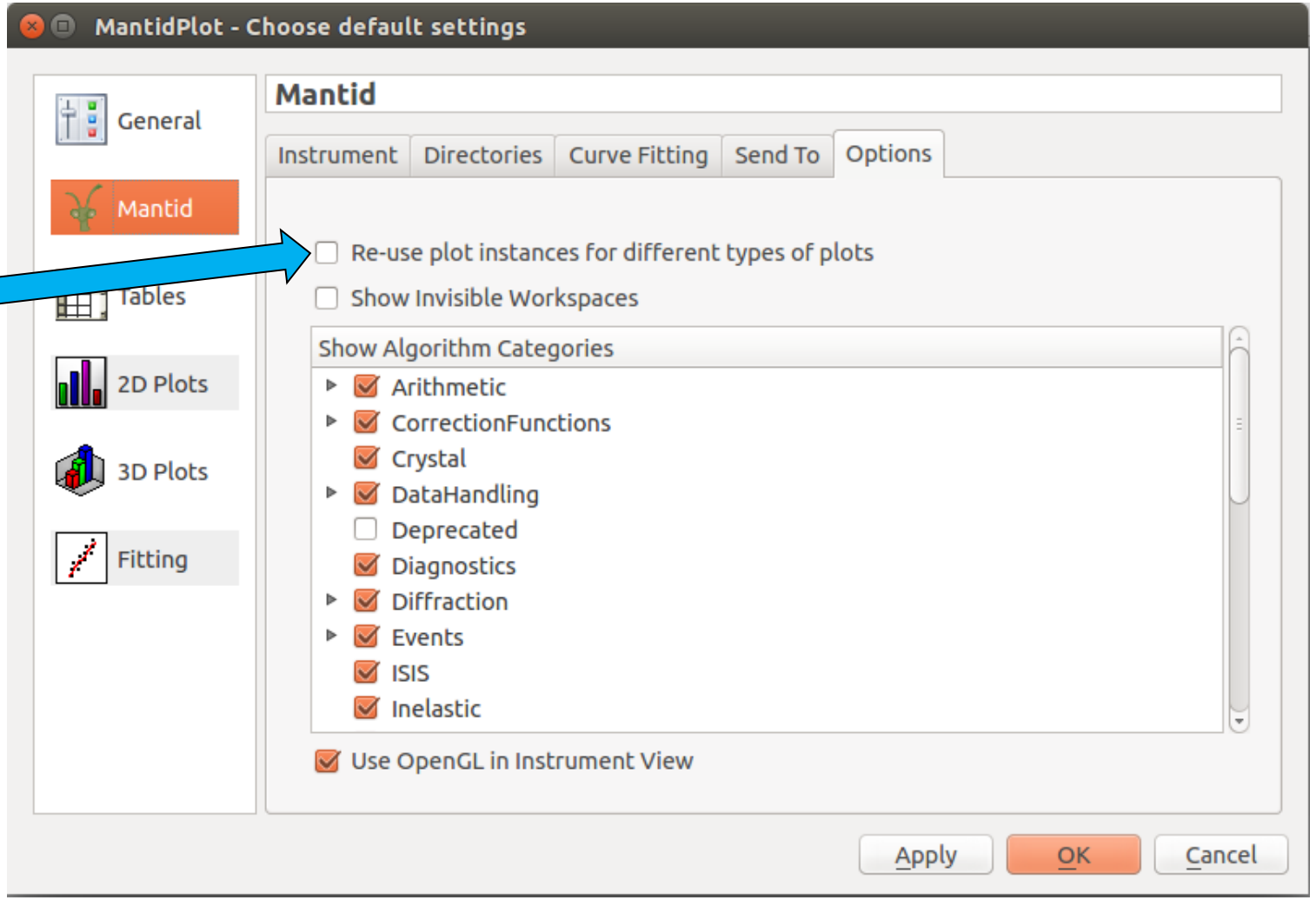
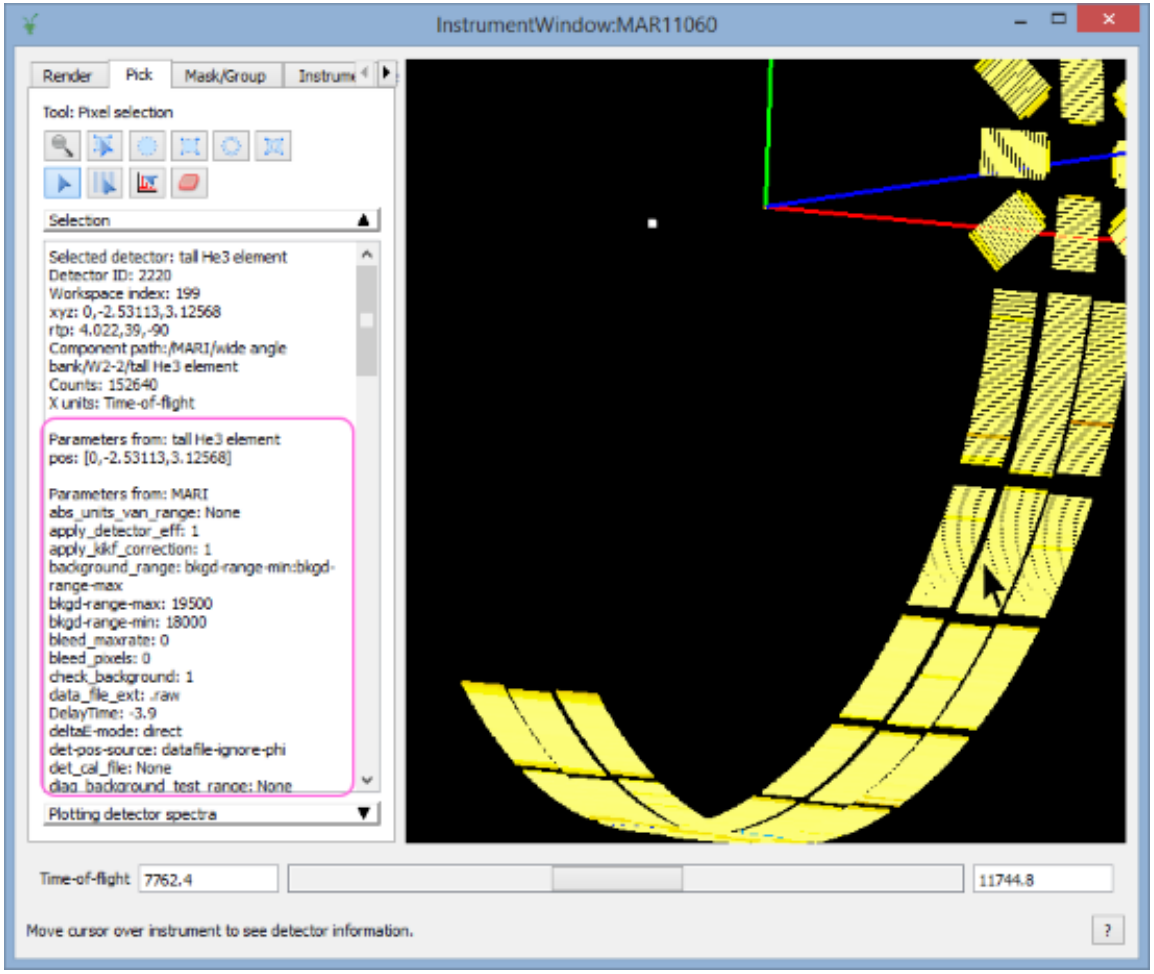
General Plot Options



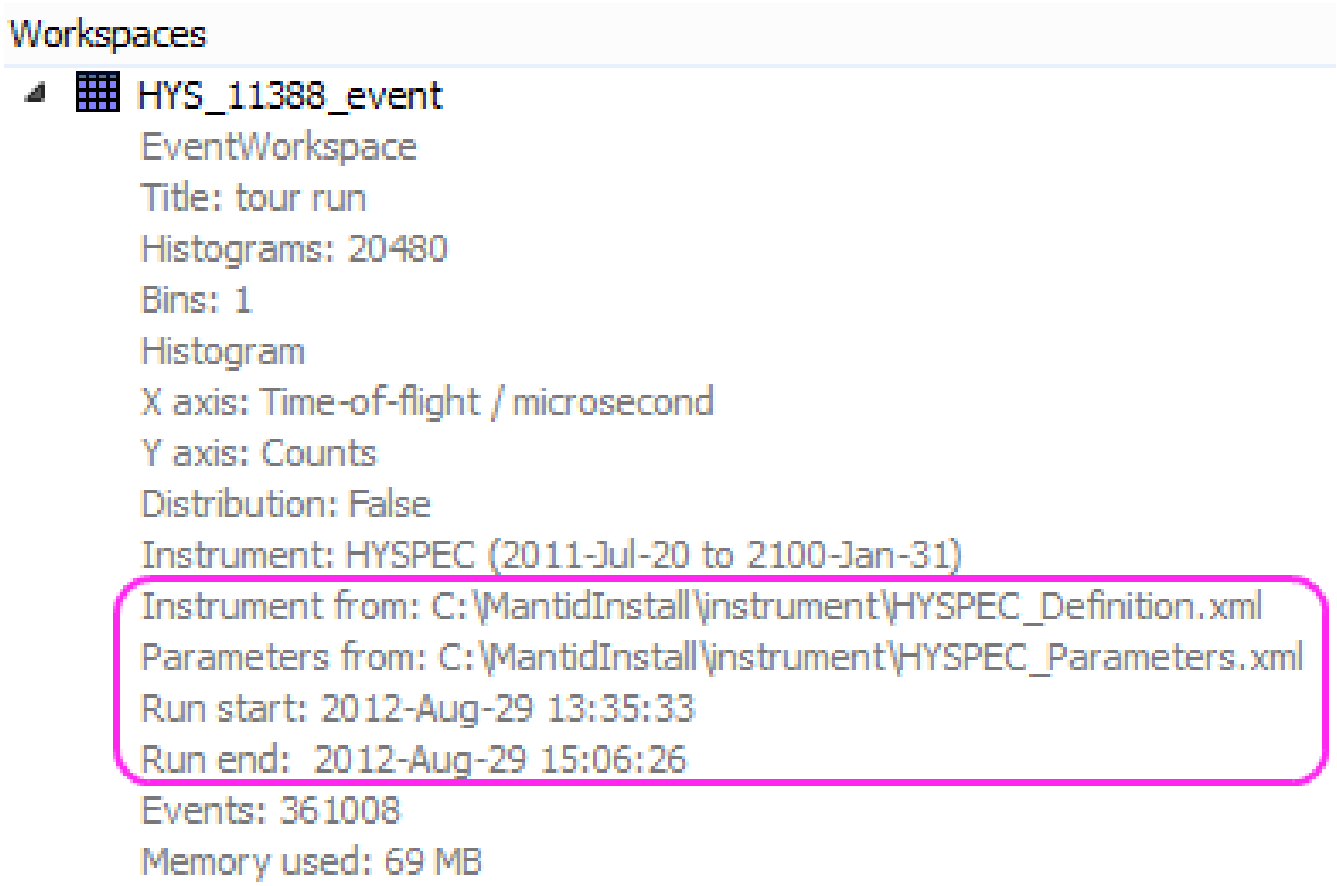
Instruments

- Instrument parameters are displayed in pick mode
- SaveParameterFile algorithm



Workspace Details

- Workspace details now display origin of instrument



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

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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…

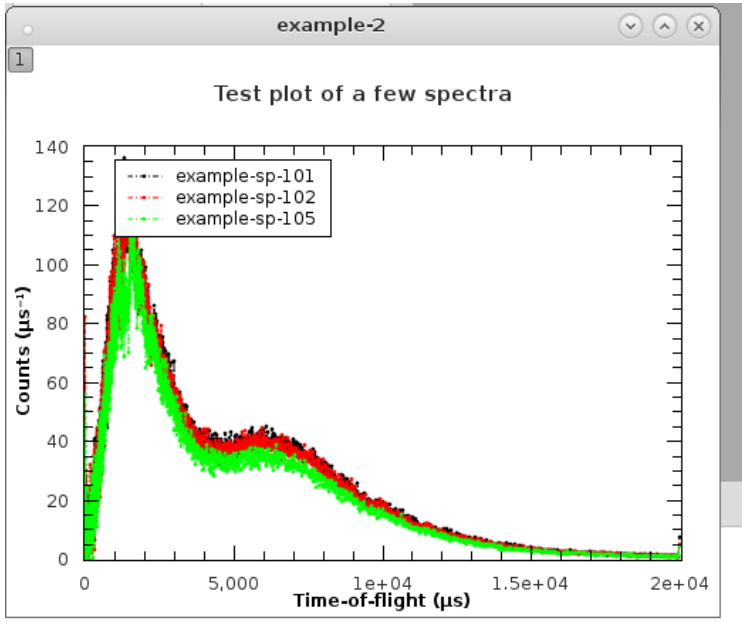
!

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

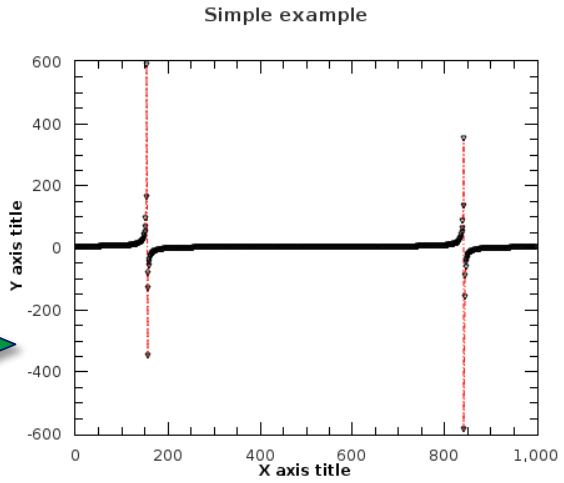
- Not to be confused:
  - Matplotlib also shipped



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')
```



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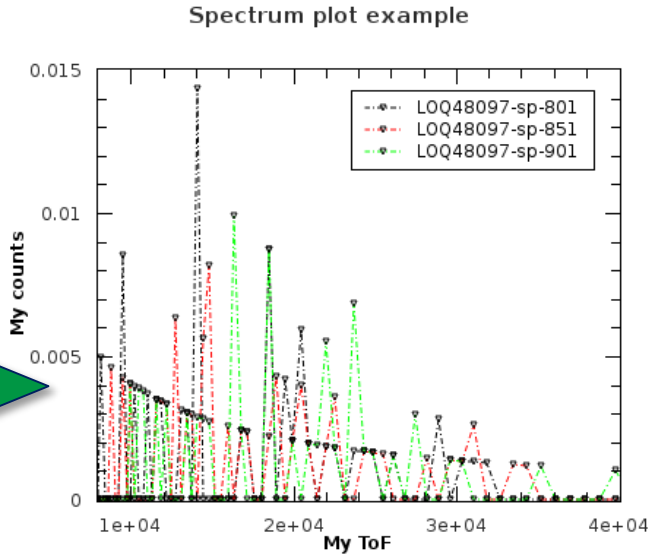
Python Command Line Interface

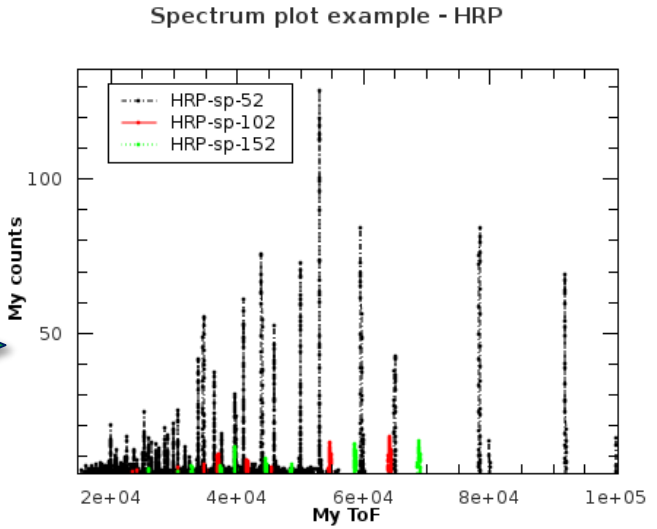
- Plotting spectra:

```
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)
```



- 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]
ax.set_ylabel('My counts')
ax.set_xlabel('My ToF')
ax.set_xlim(1.5e4, 1e5)
ax.set_ylim(5, 135)
```



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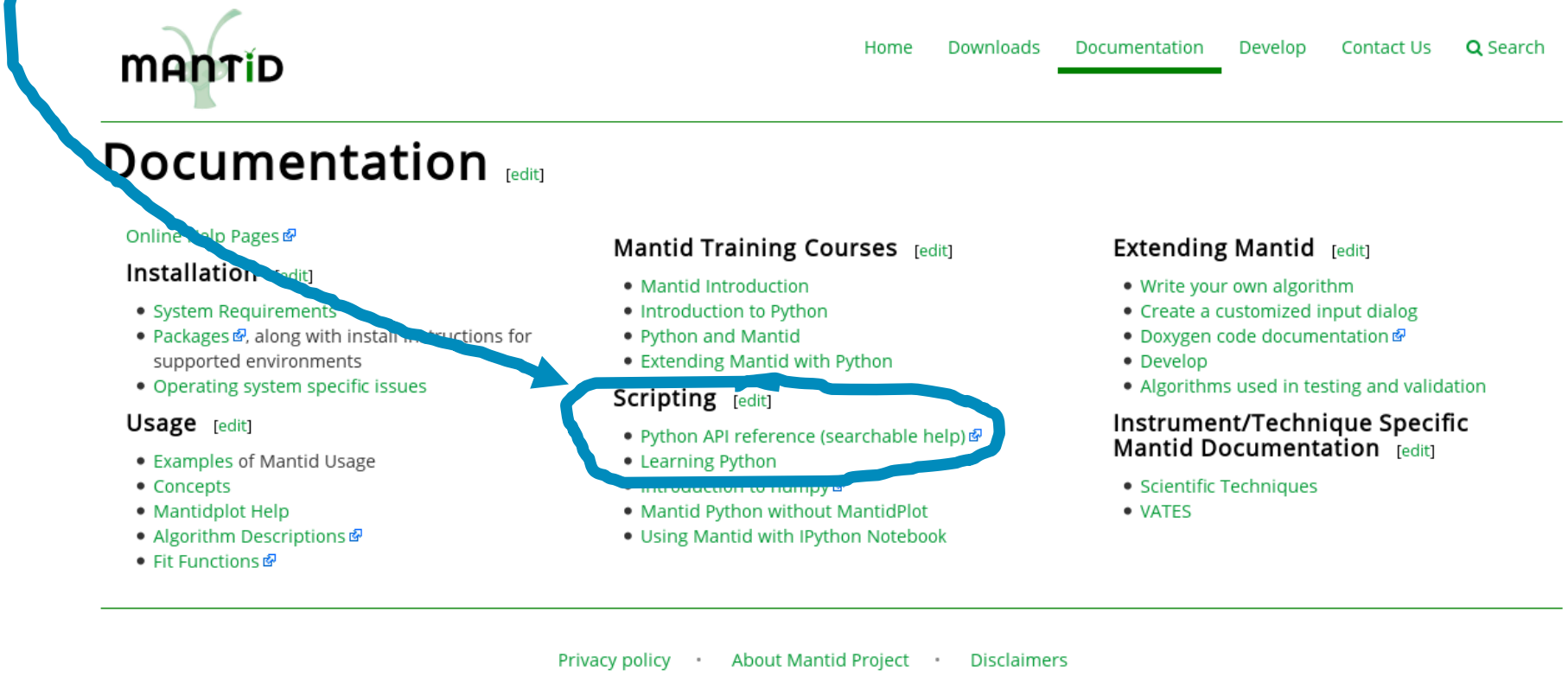
Python Command Line Interface

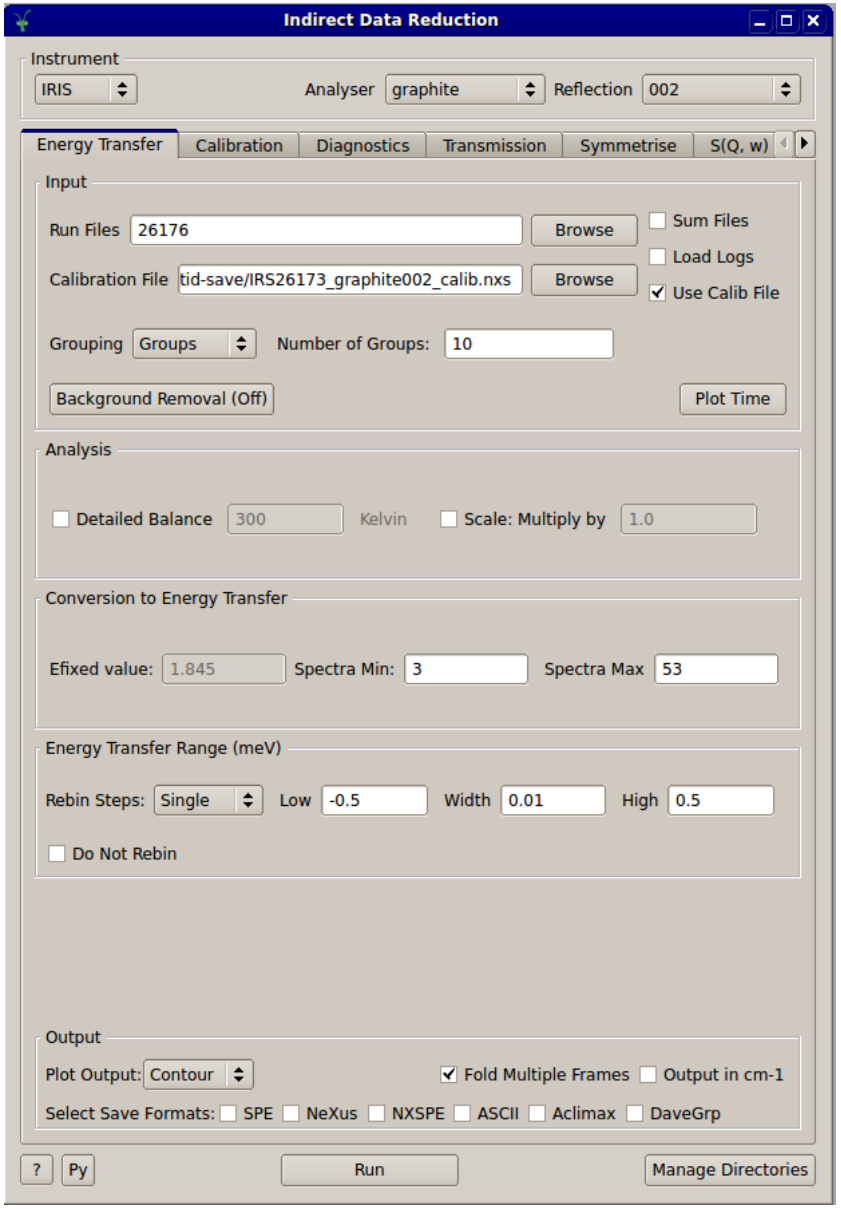
- To learn how to use it:
  - help(pymantidplot.future.pyplot)
  - http://docs.mantidproject.org/nightly/api/python/index.html
  - Familiar interface, >90% like the Pyplot tutorial: http://matplotlib.org/users/pyplot_tutorial.html



Indirect Inelastic

Updates to Interfaces

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



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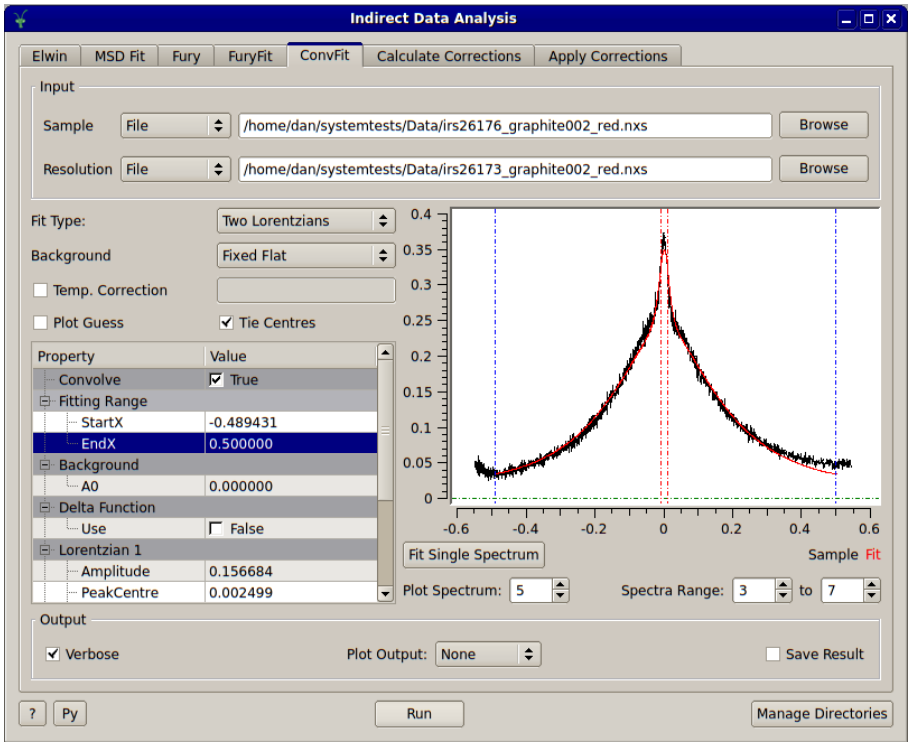
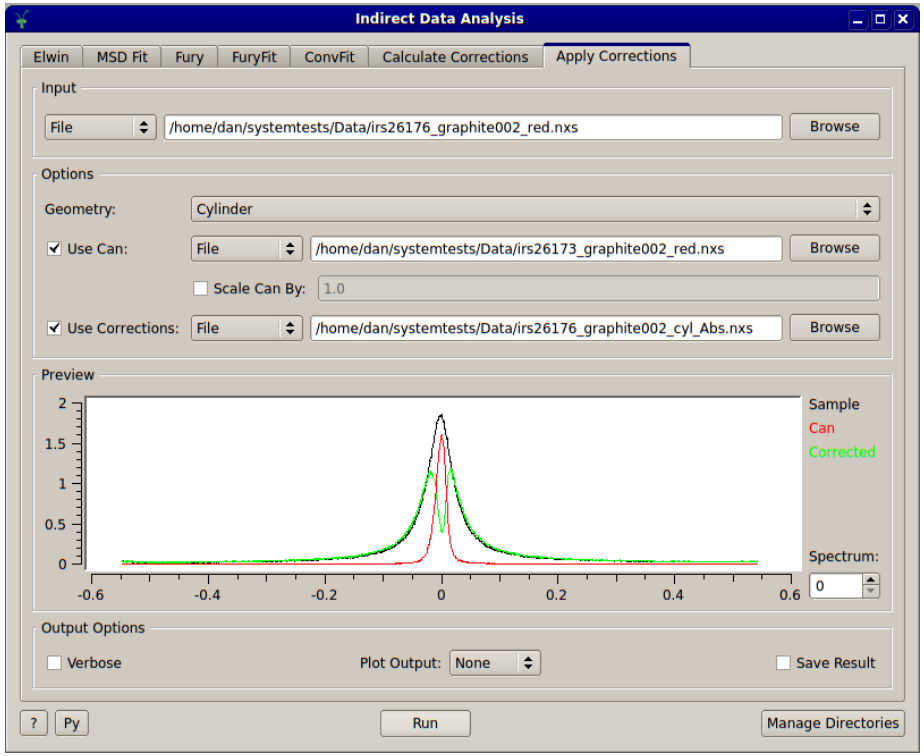
Updates to Interfaces

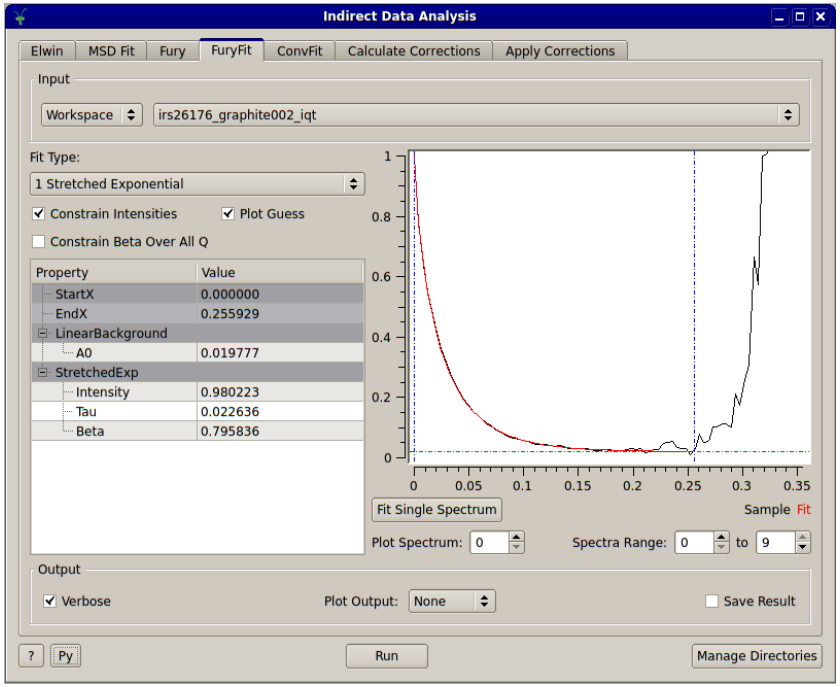
- Preview plots and spectra selection
- S(Q, w) support on IDR and Bayes

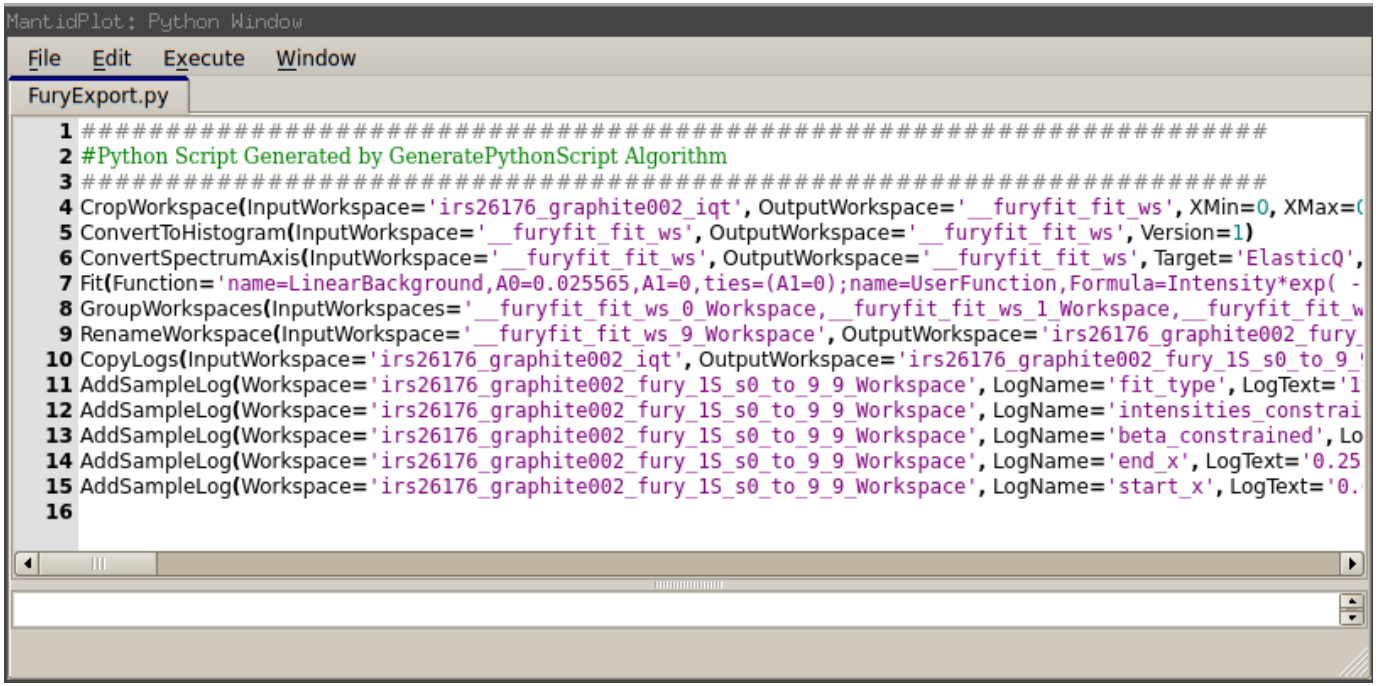




Updates to Interfaces

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





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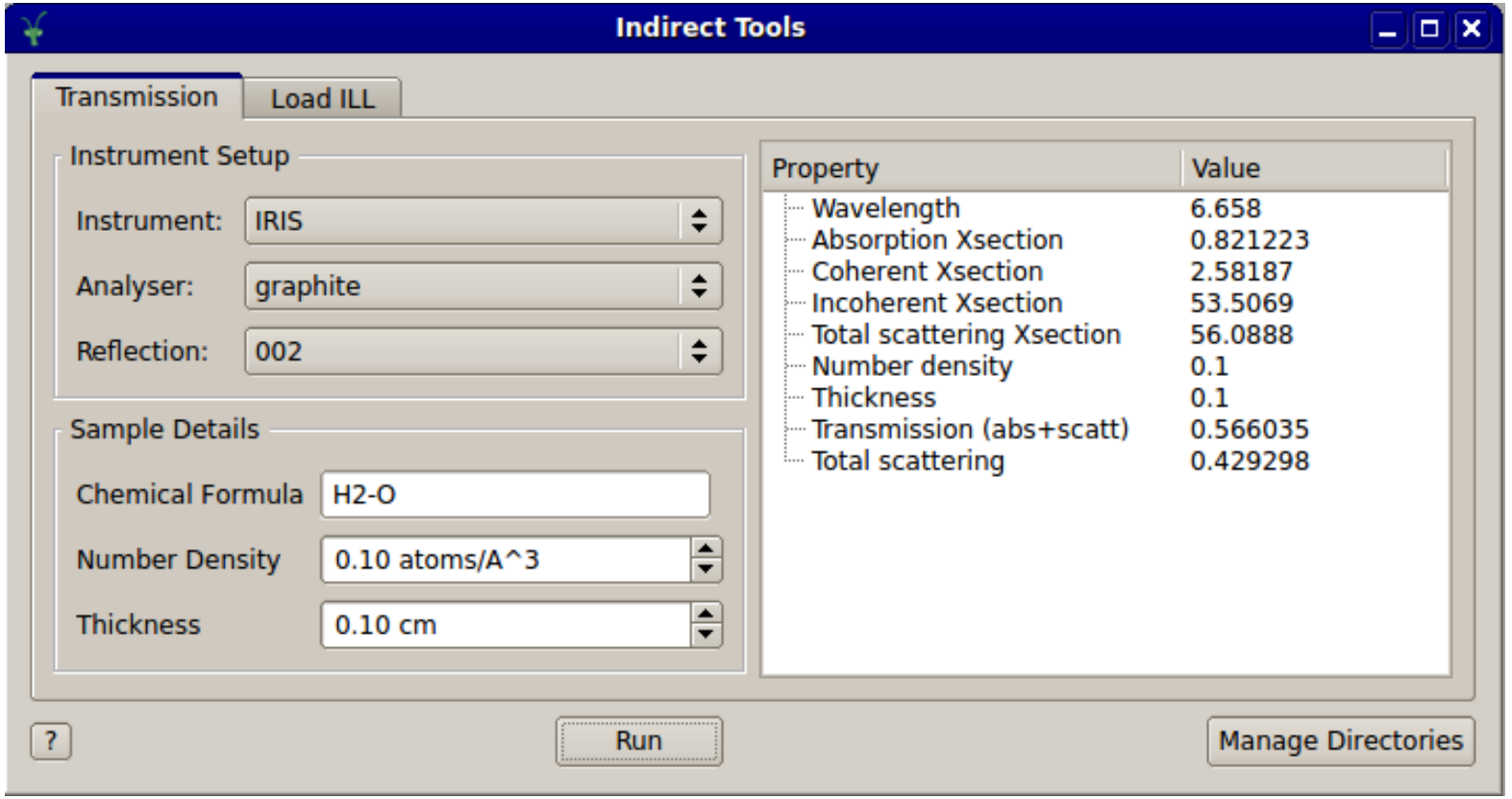
New Interfaces

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



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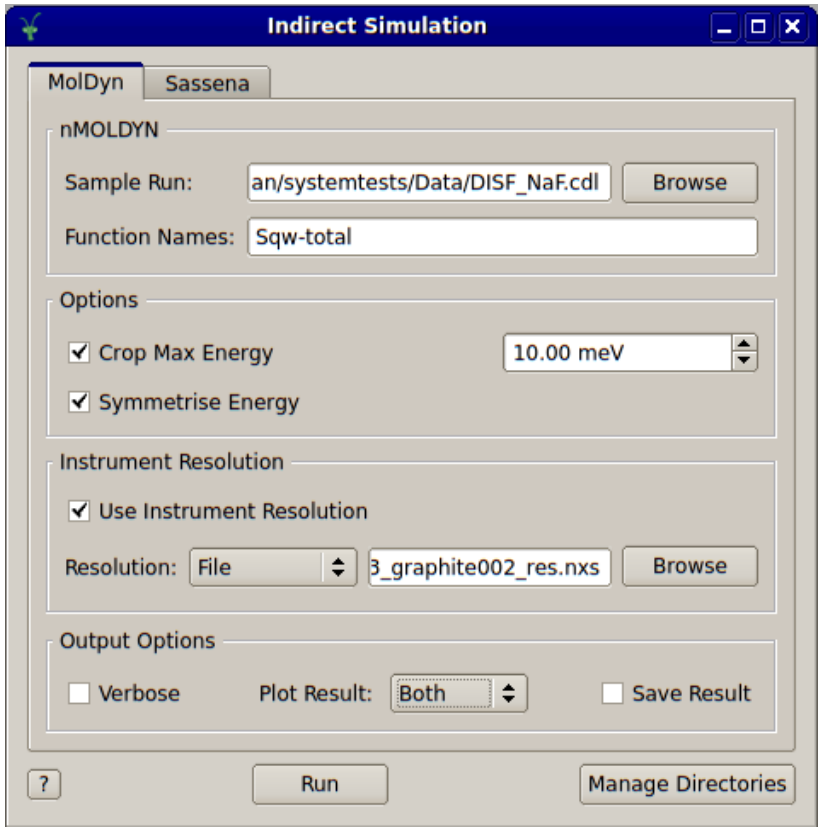
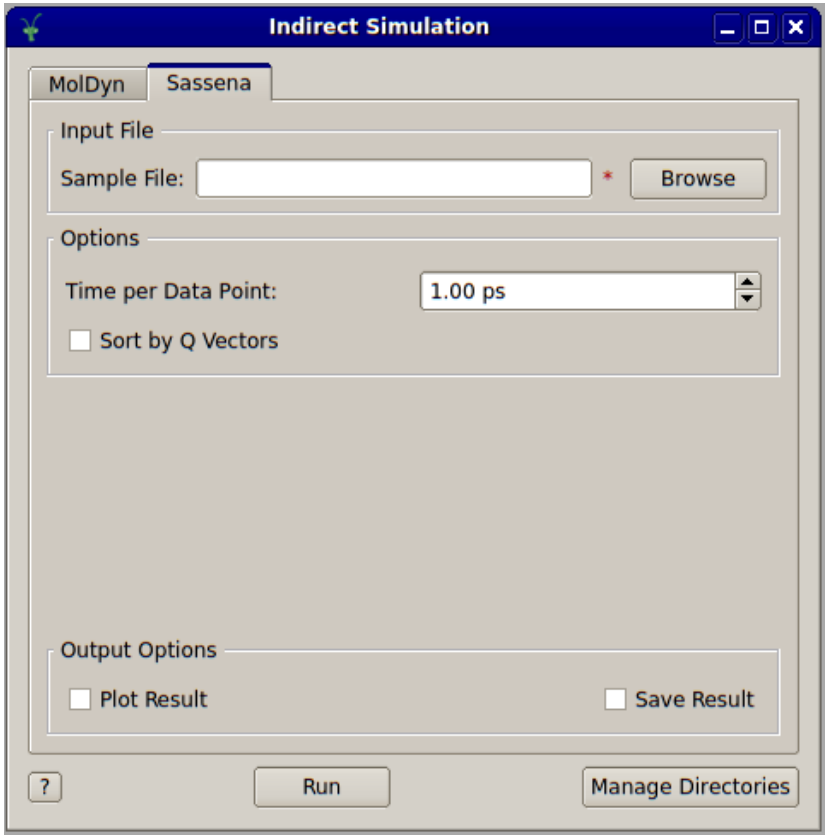
New Interfaces

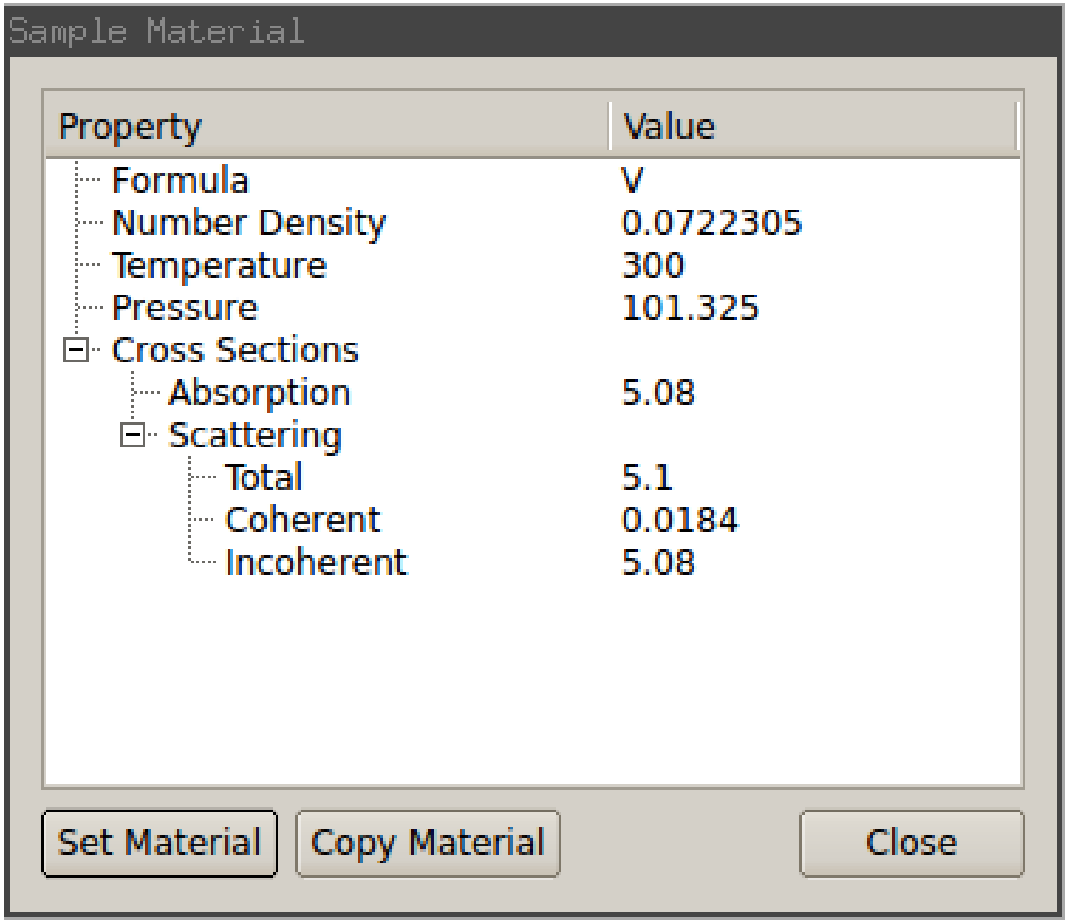
- Simulation, currently contains loaders for nMOLDYN and Sassena data





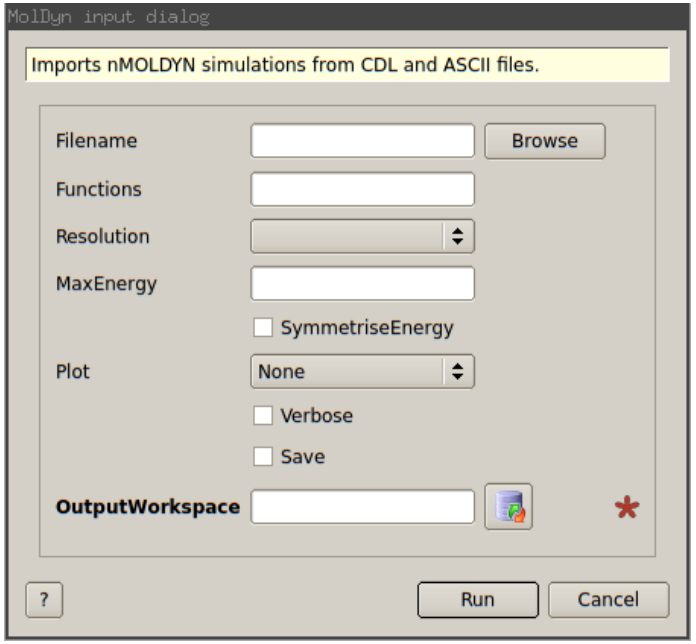
New Interfaces

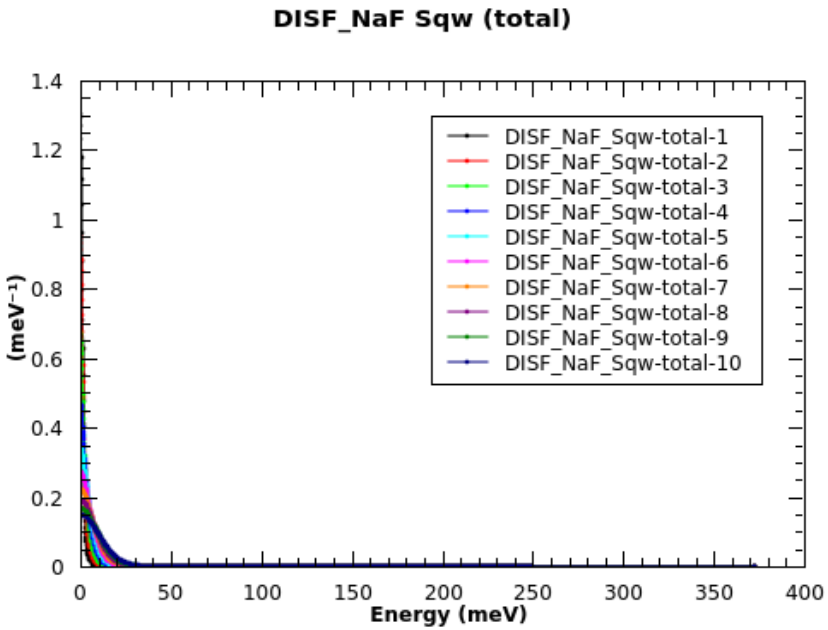
- Sample material UI
  - Show properties of sample material for a given workspace

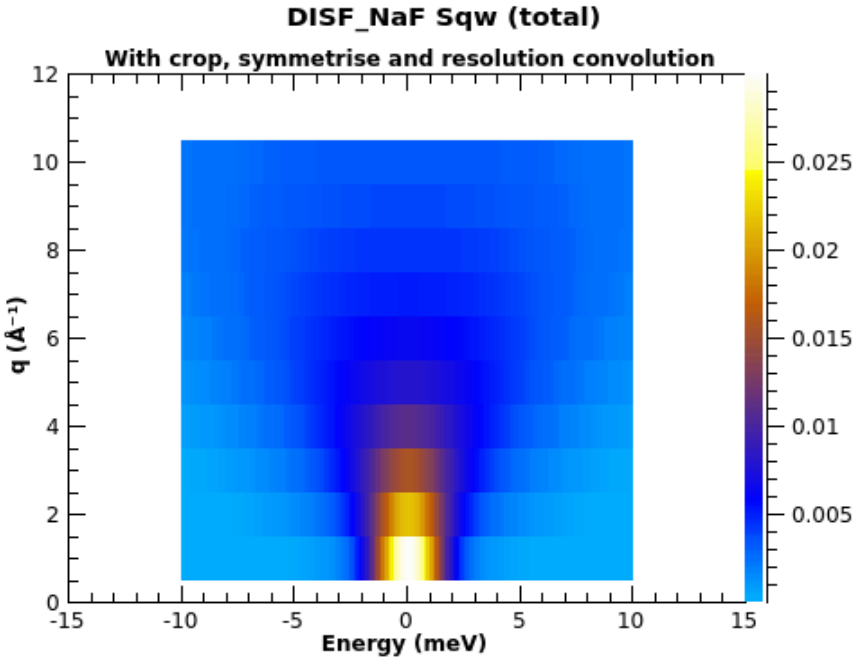


Simulation

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







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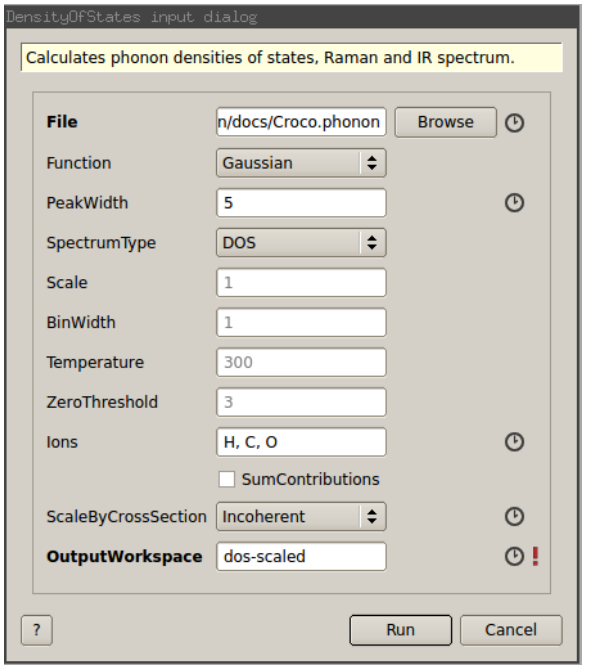
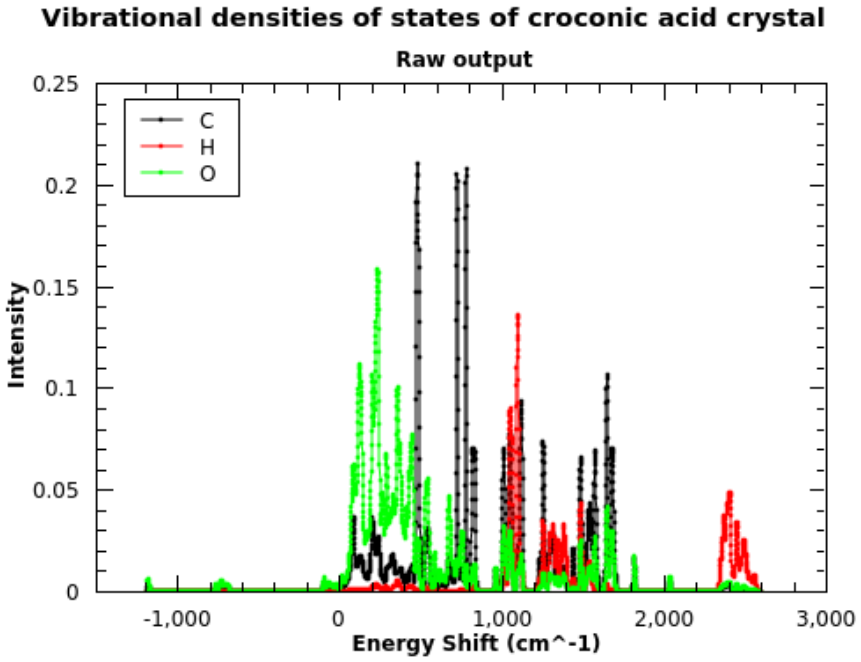
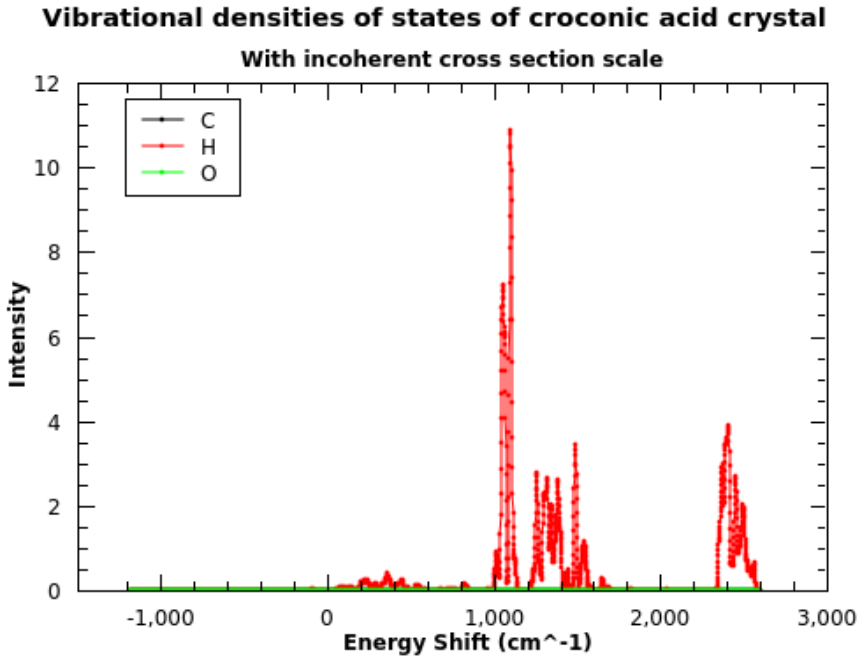
Simulation

- Scattering cross section scaling in DensityOfStates







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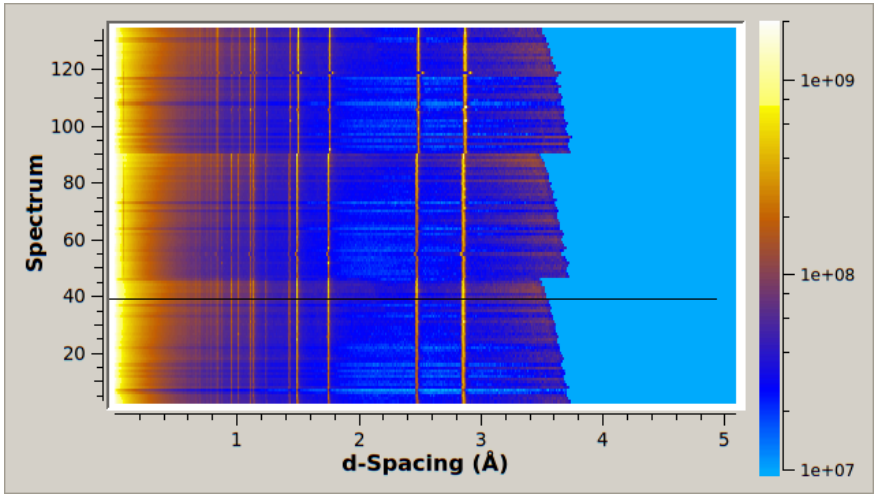
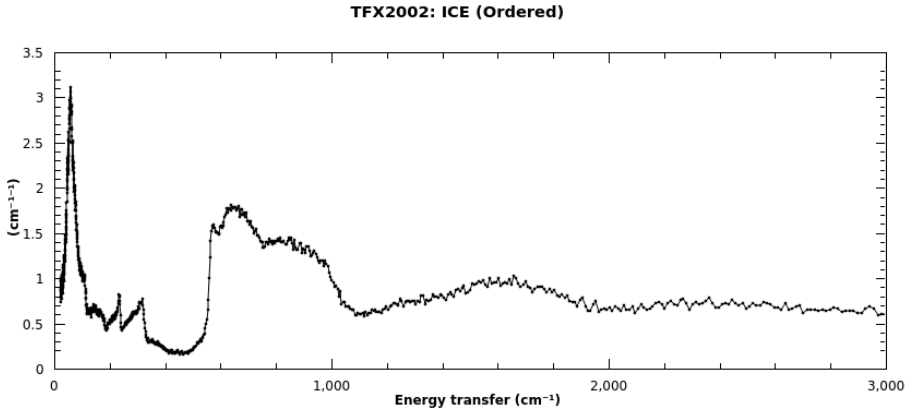
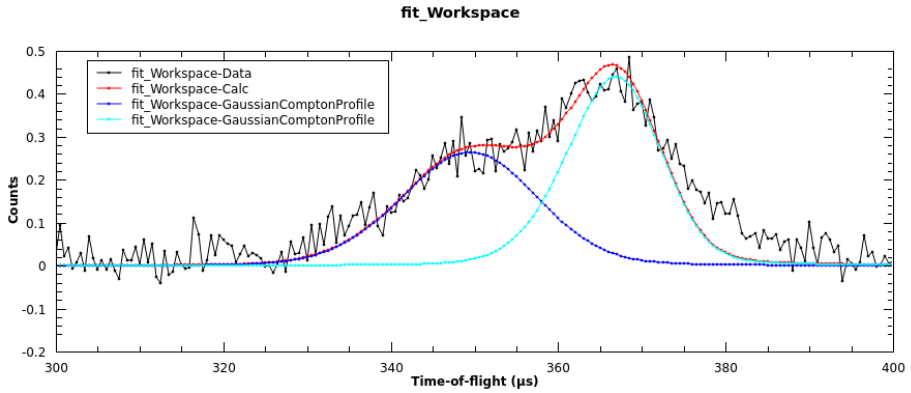
Instrument Support

- 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







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Reflectometry

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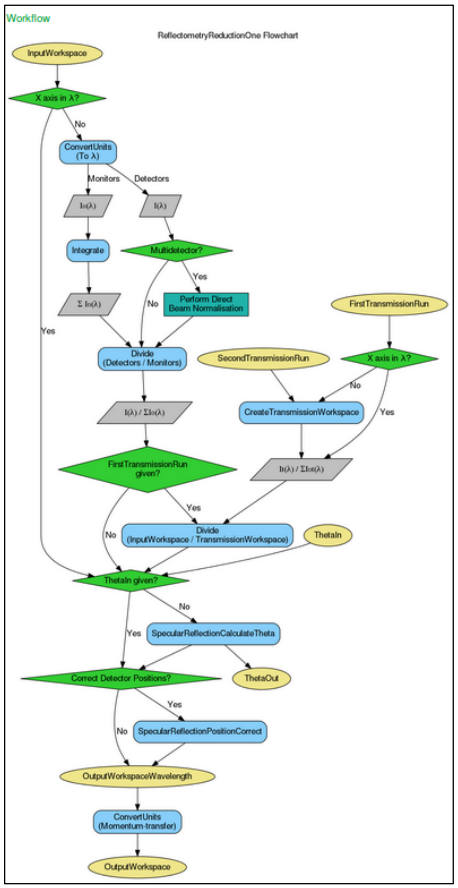
Algorithms

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



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

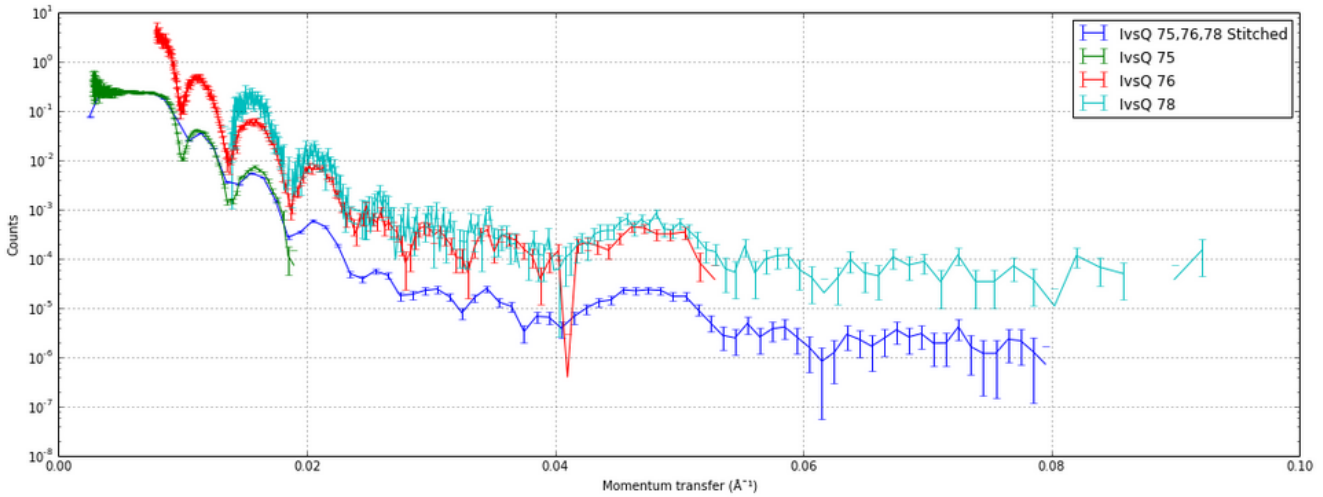
Code | Cell Toolbar: None

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 (Å$^{-1}$)")
axes.set_ylabel("Counts")
axes.set_yscale("log")
```



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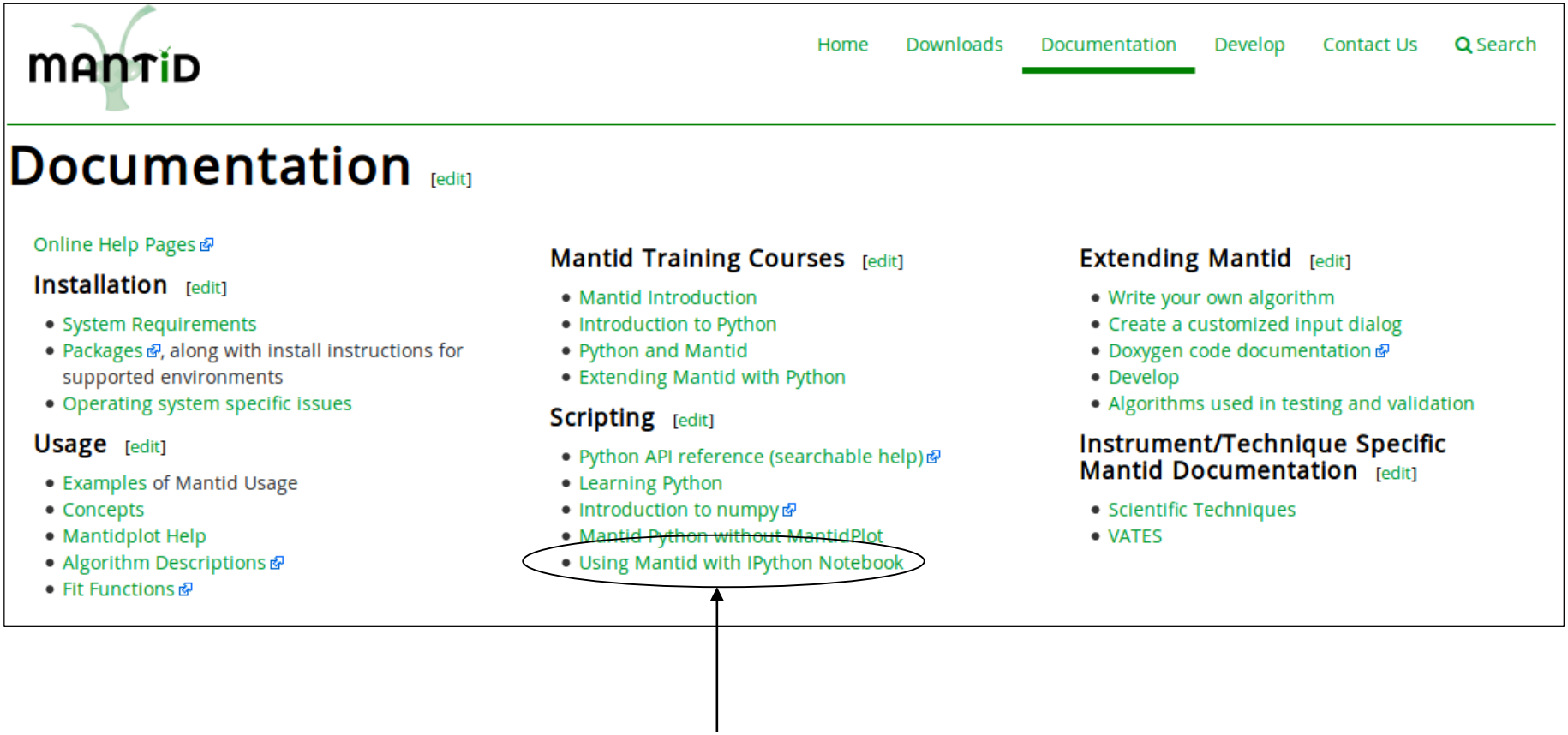
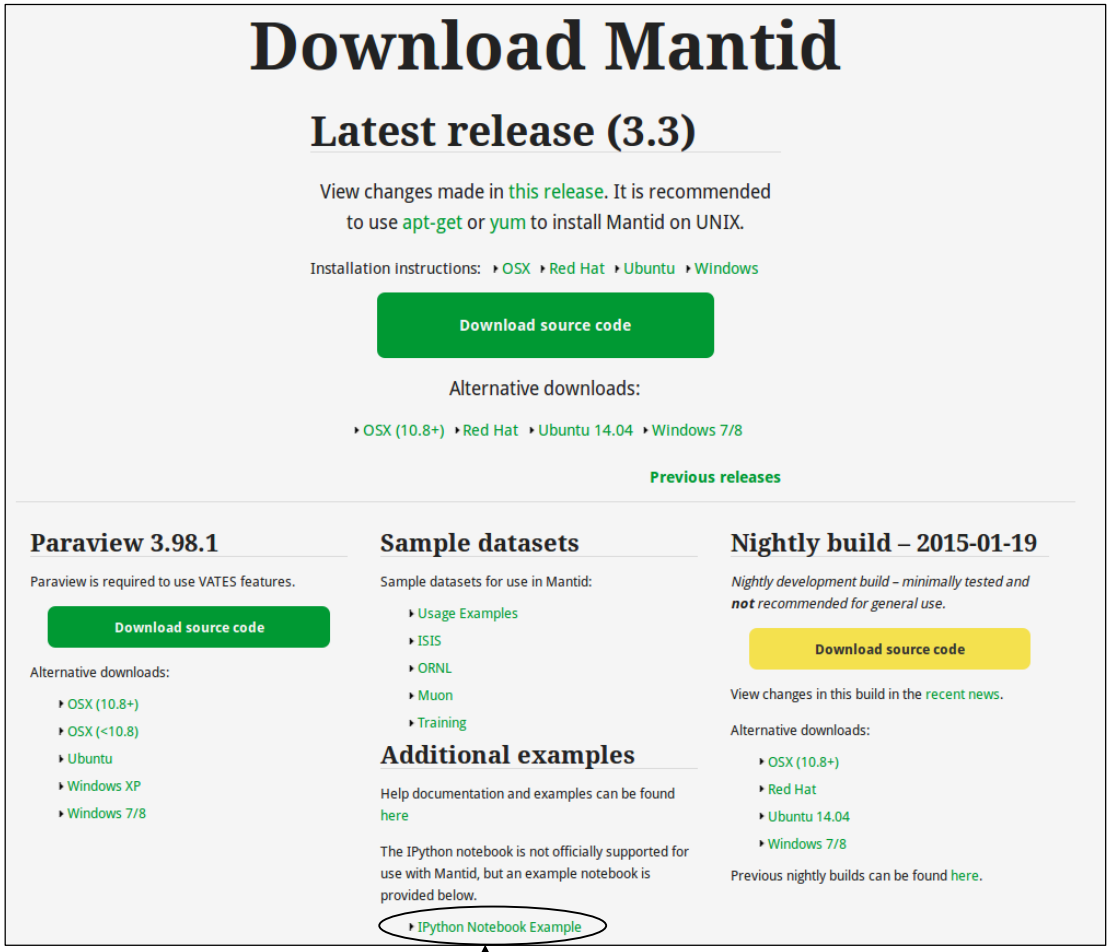
Experimental IPython Notebook Support



Using Mantid with IPython Notebook

Experimental IPython Notebook Support



IPython Notebook Example

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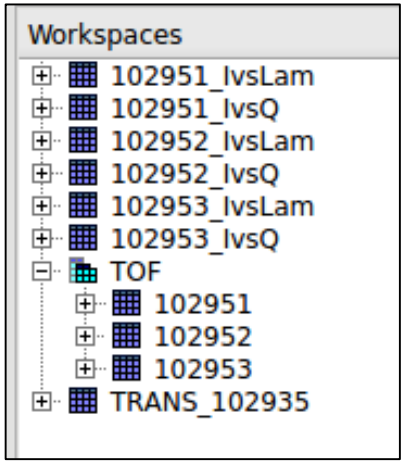
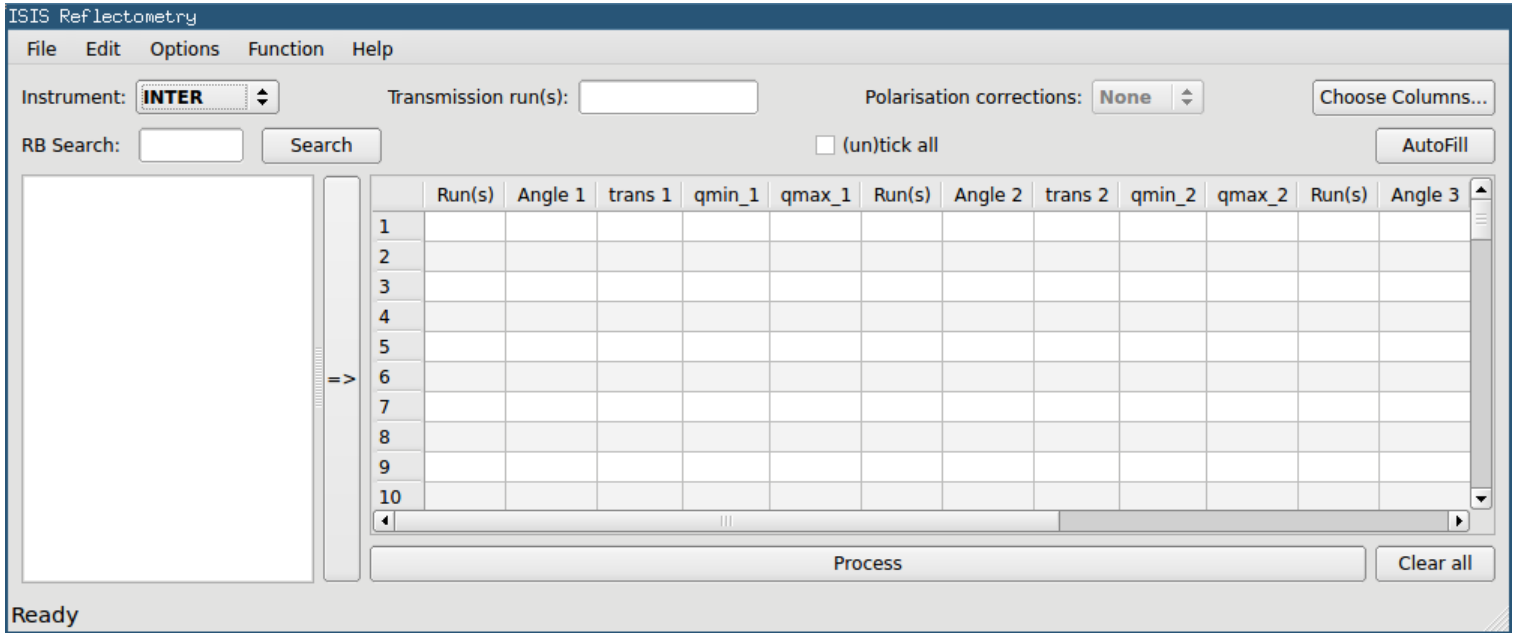
Reflectometry – ISIS Reduction Interface

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





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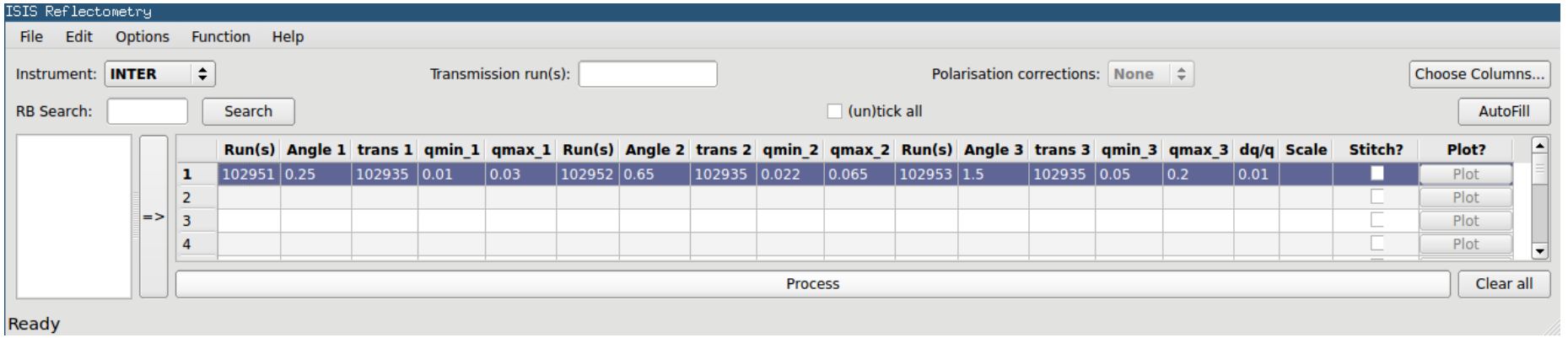
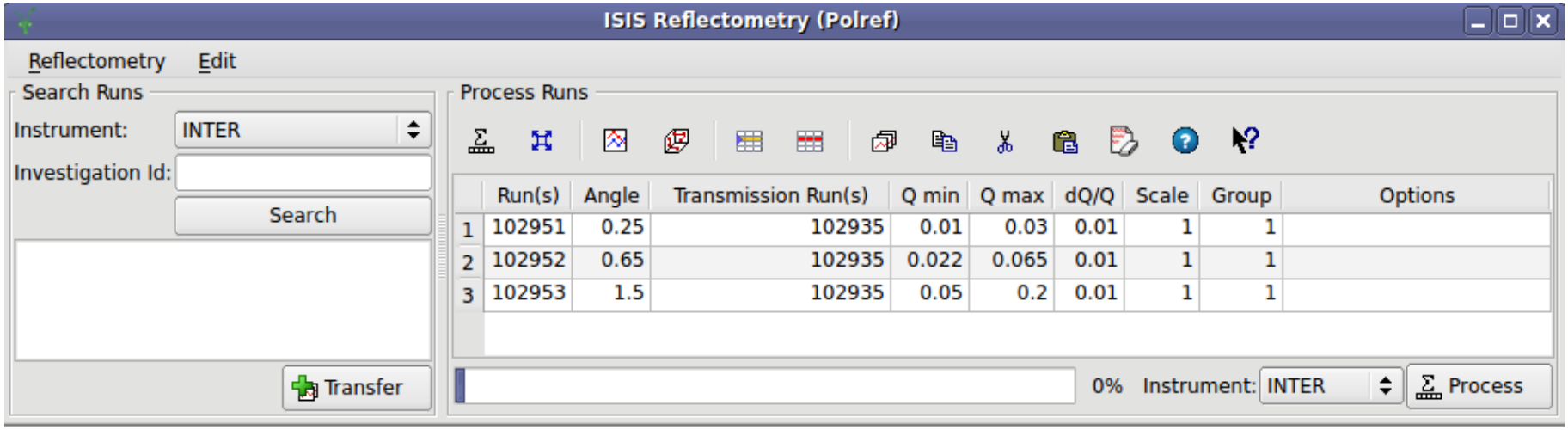
Reflectometry – New Reduction Interface

Existing UI



New UI



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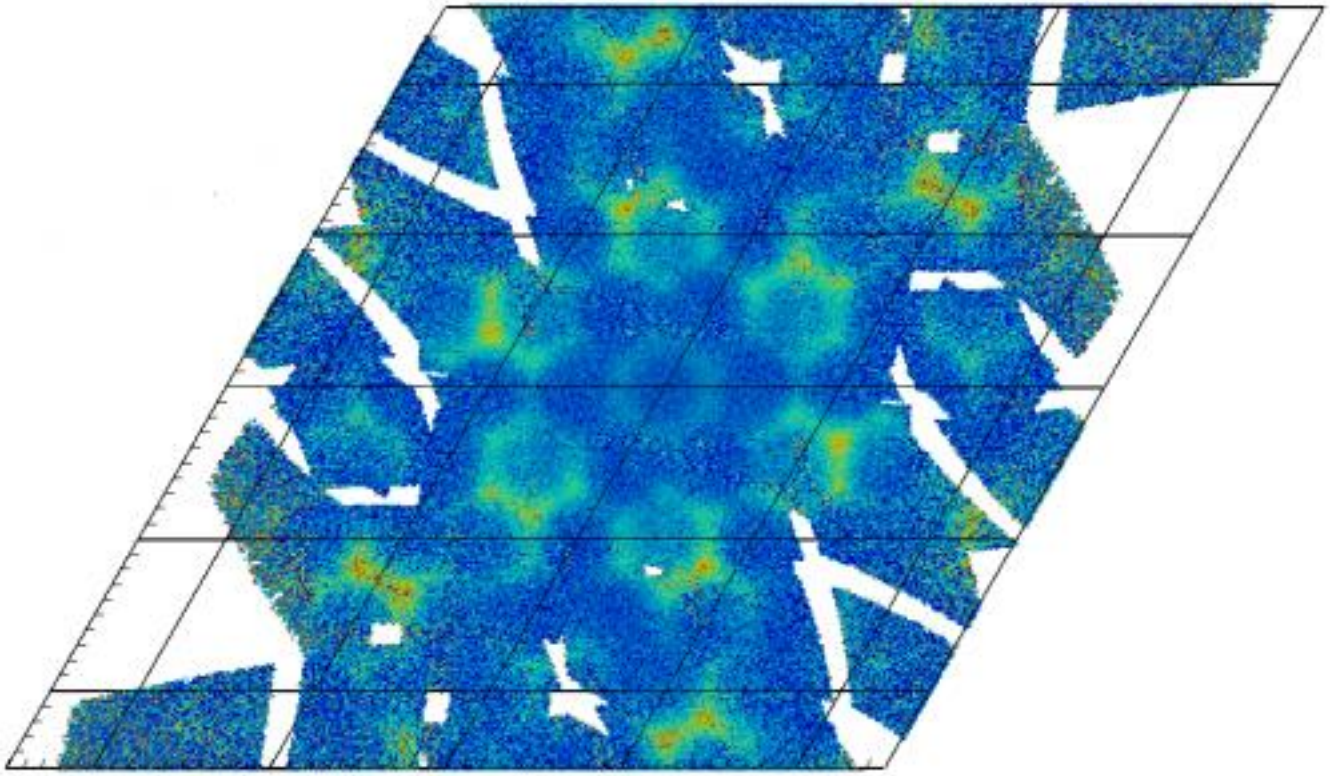
Reflectometry – New Reduction Interface

Demo

Diffraction

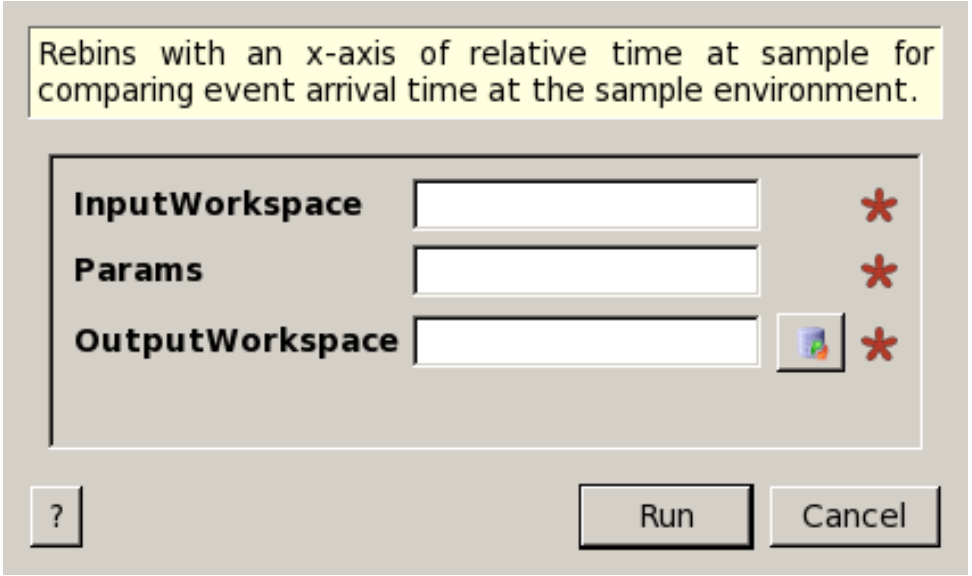
Normalisation

- 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**



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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
```

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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	$\bar{1}$

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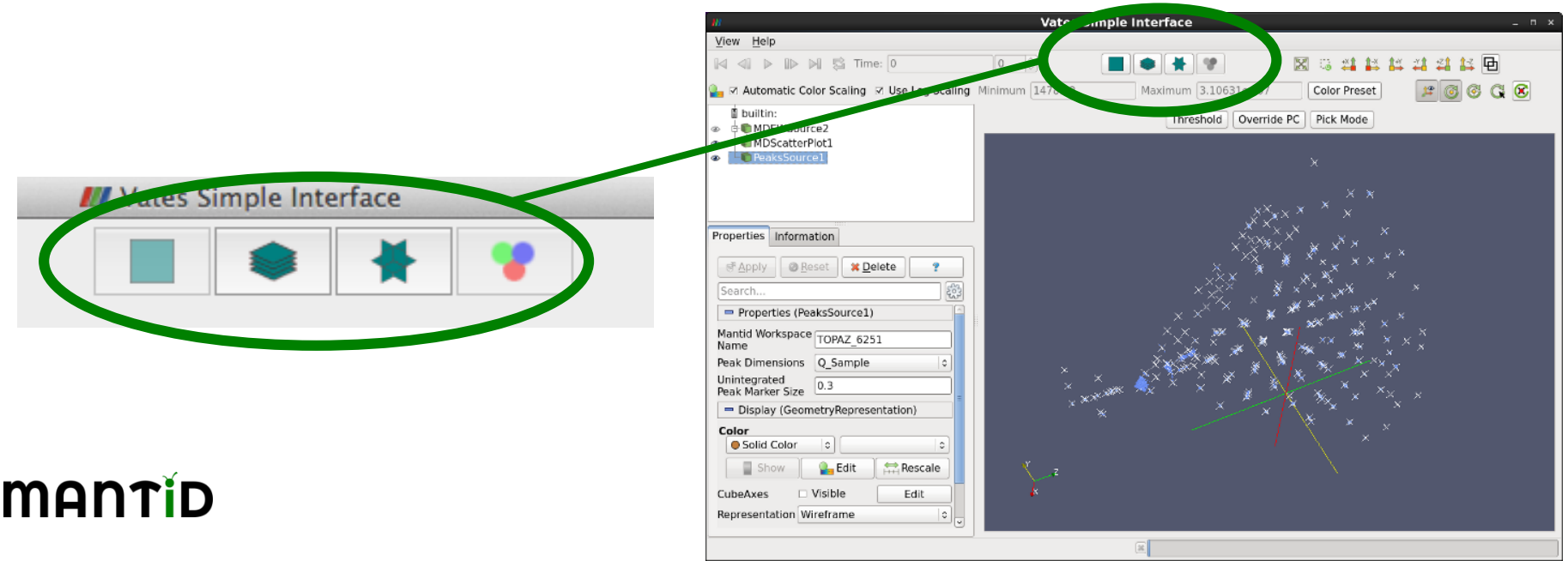
Fixes and Improvements

- **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



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SANS

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SANS

http://www.mantidproject.org/ISIS_SANS

- SANS user file commands
- Compatibility of different web browsers with canSAS XML data files /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

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

where

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

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

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

Muon

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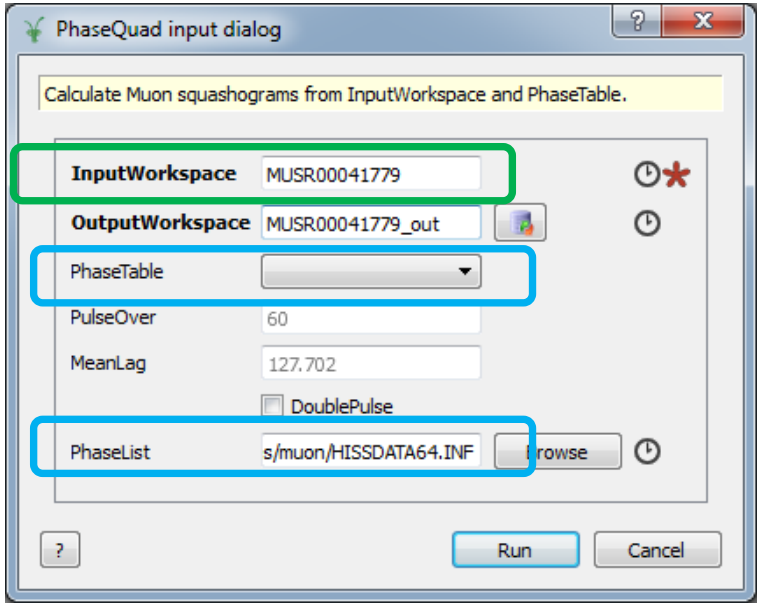
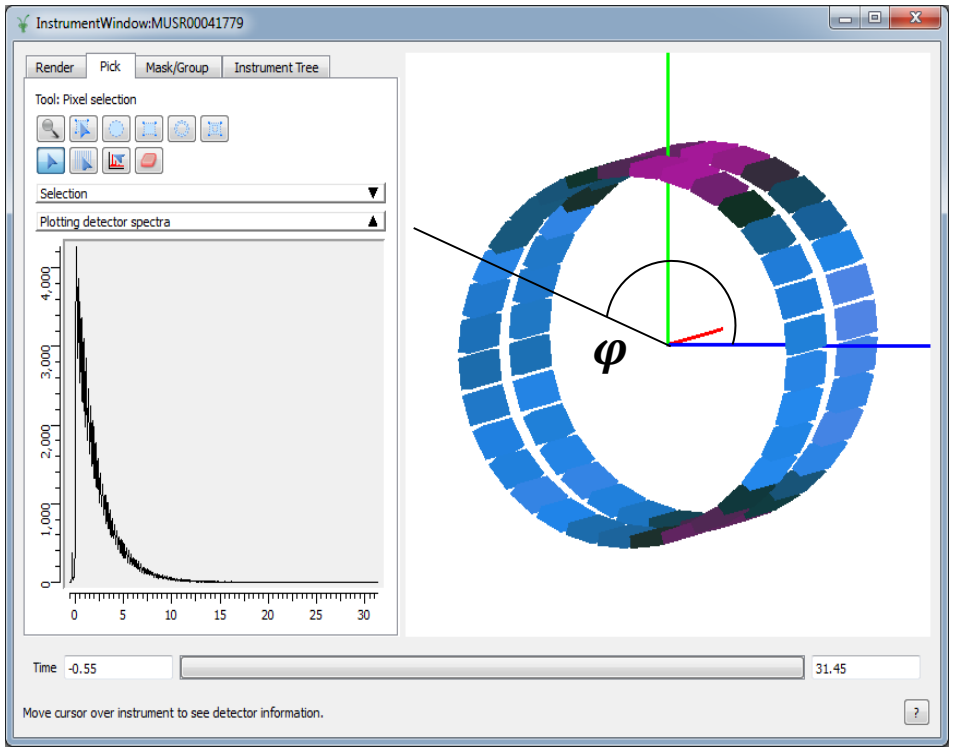
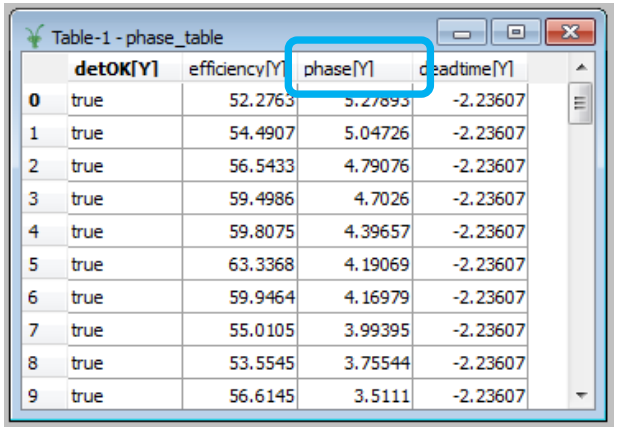
Muon

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



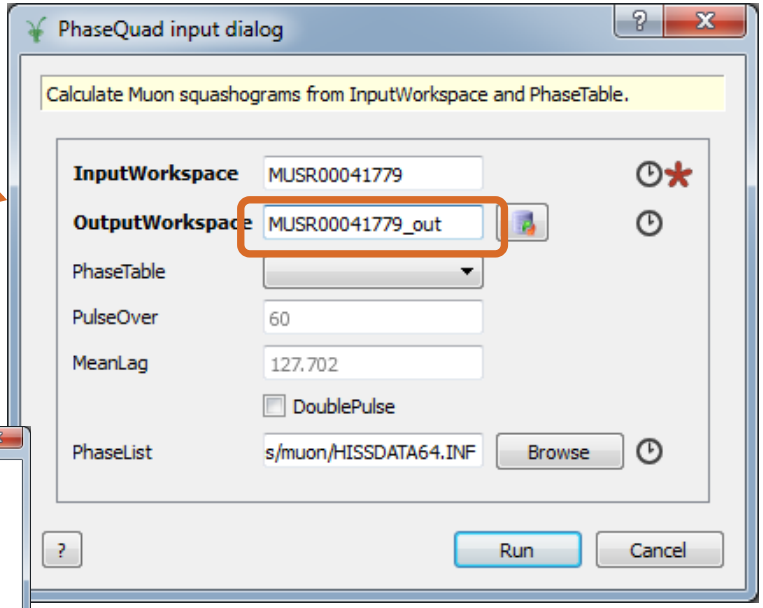


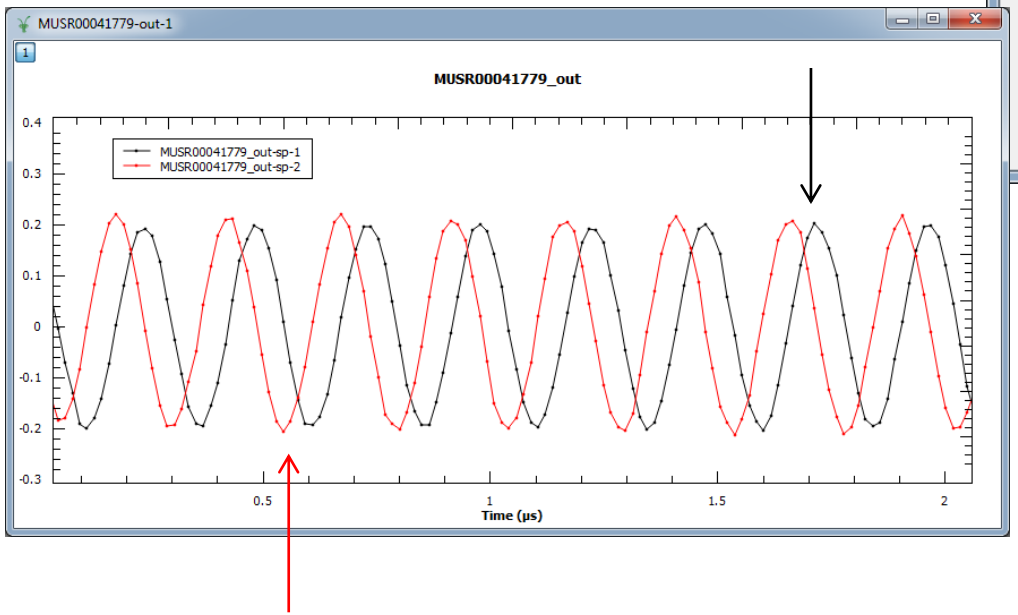
  - Input **phase** table/list

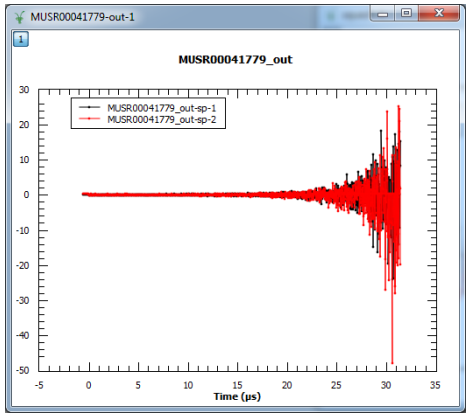


Muon

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







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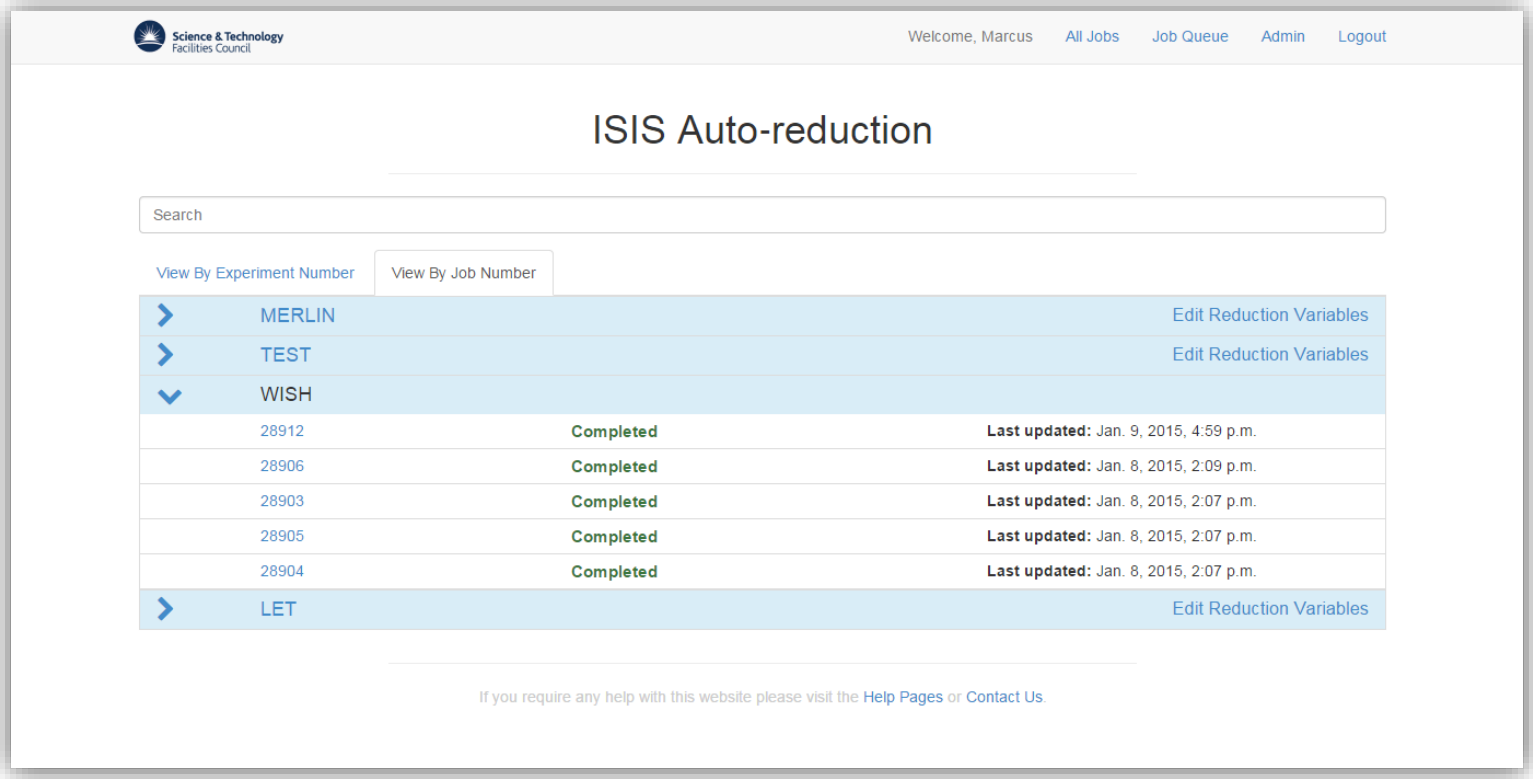
Autoreduction

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.



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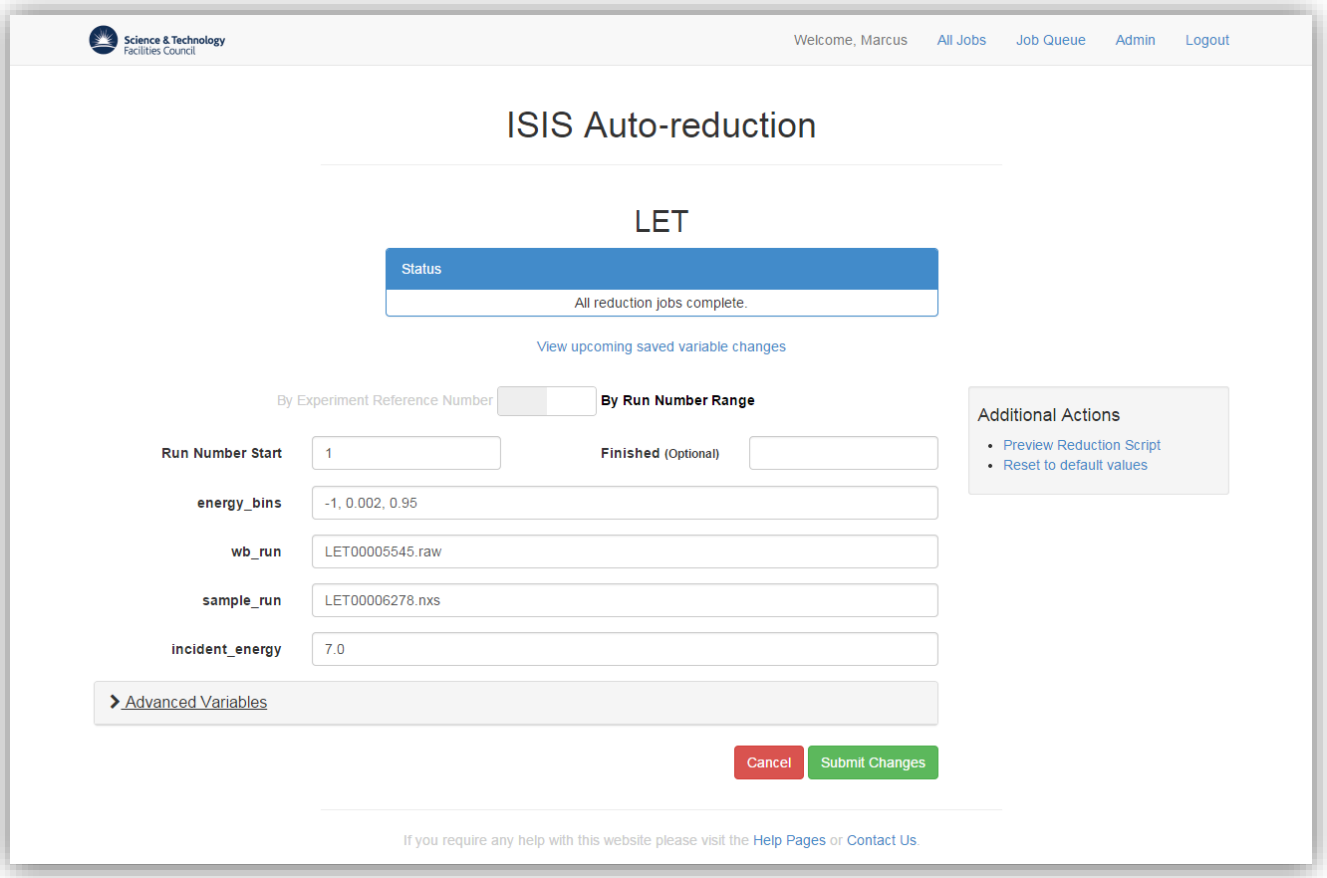
** Added by Instrument Scientist*

Features

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



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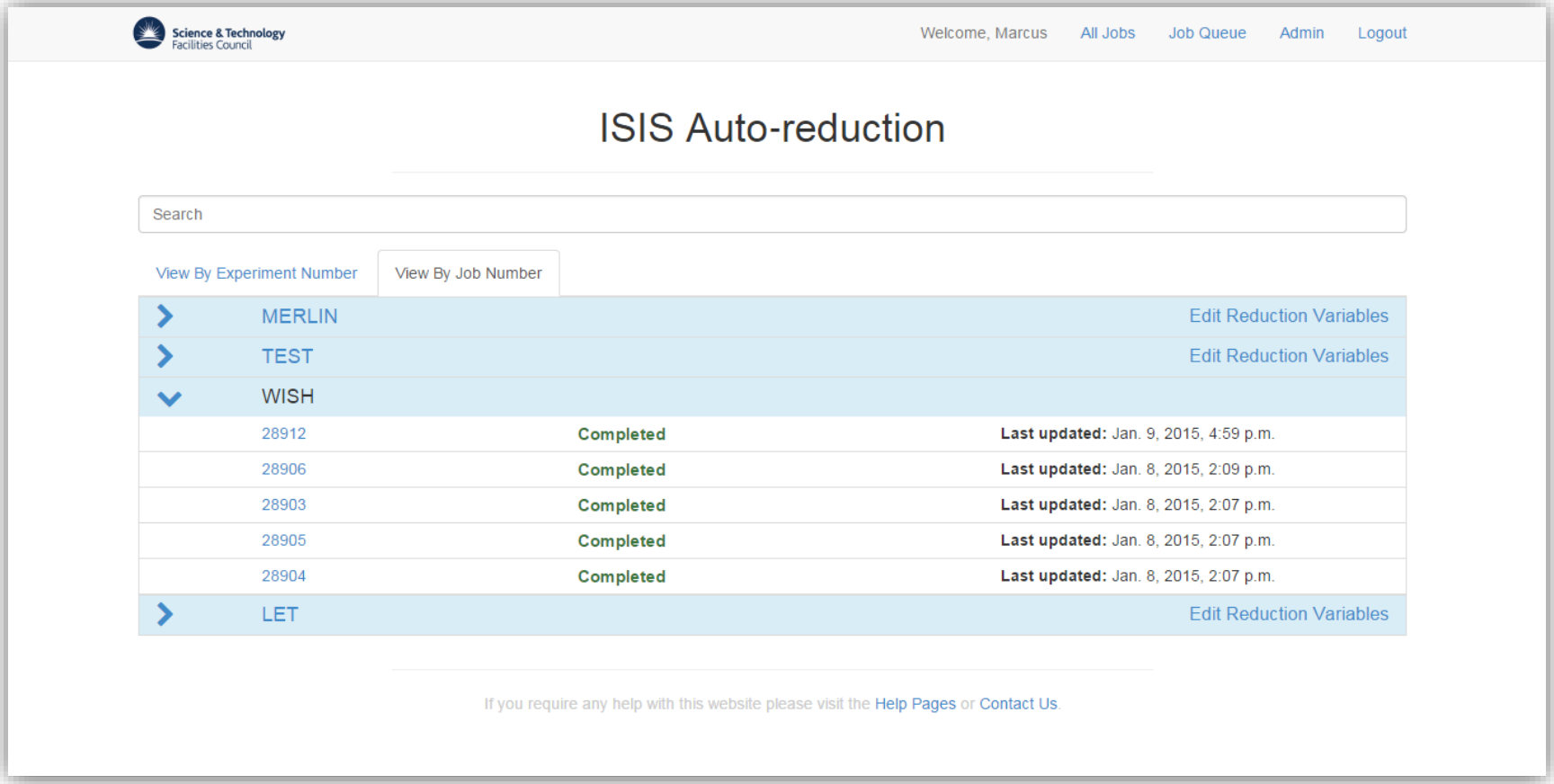
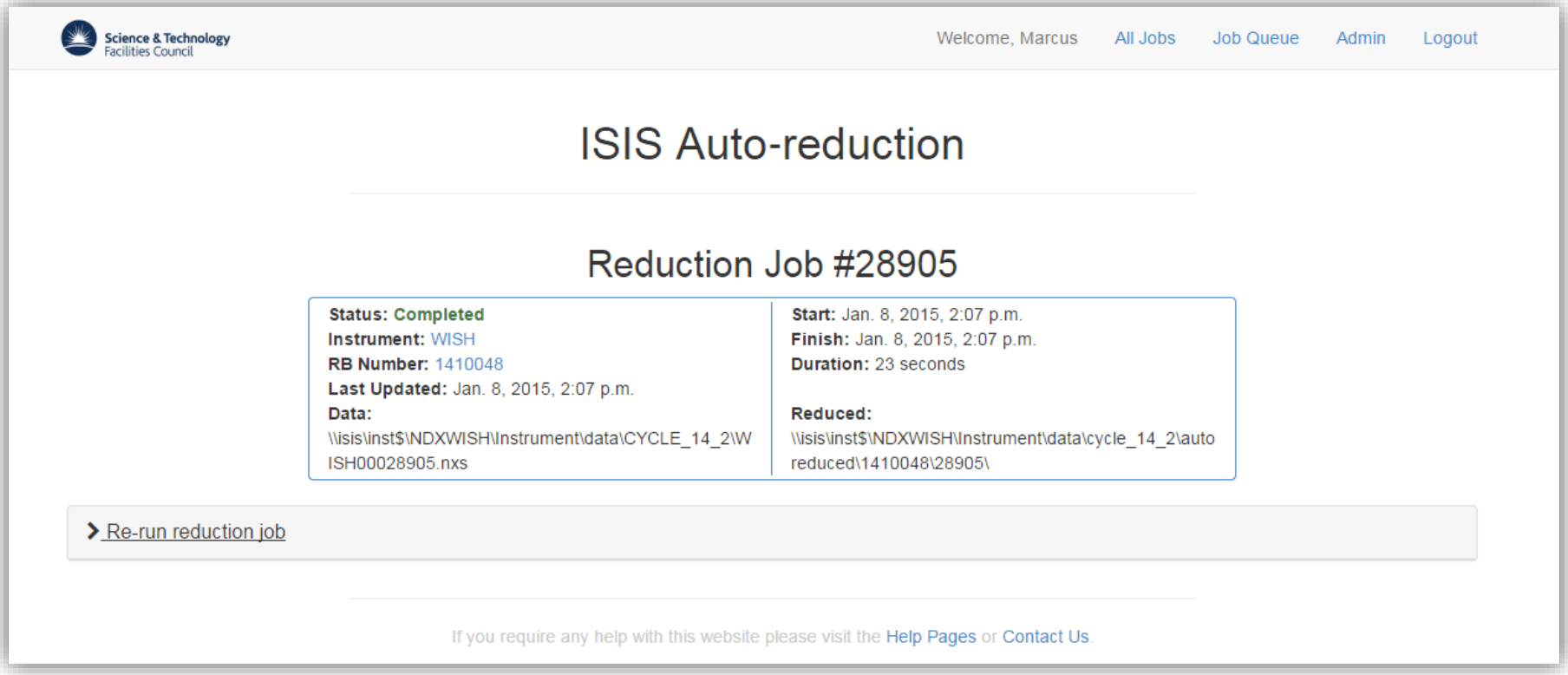
Features

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



Features

- View details of each run.



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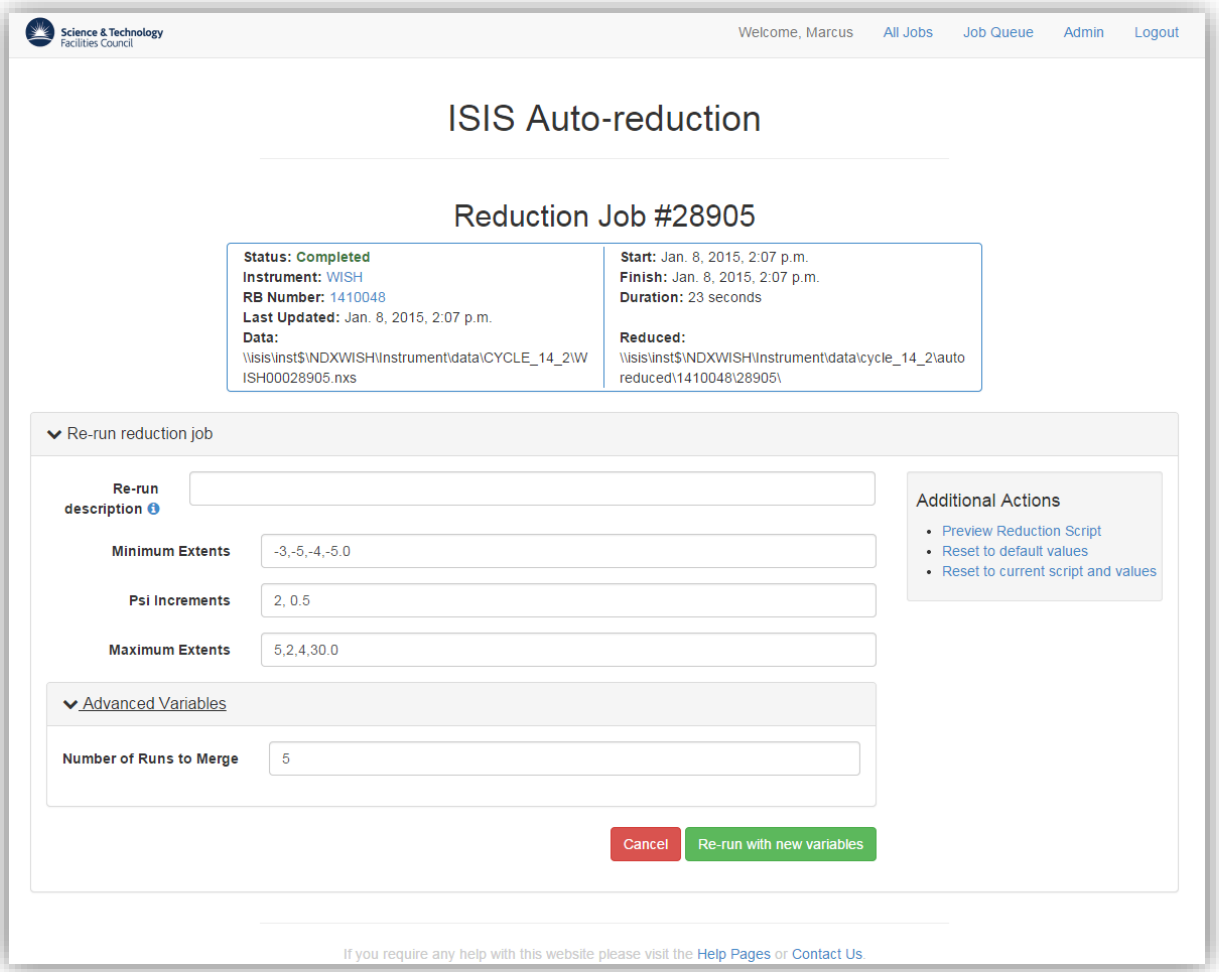
Features

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



Features

- Access it from many devices.

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Demo

(*Hopefully*)

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System Problems / Help

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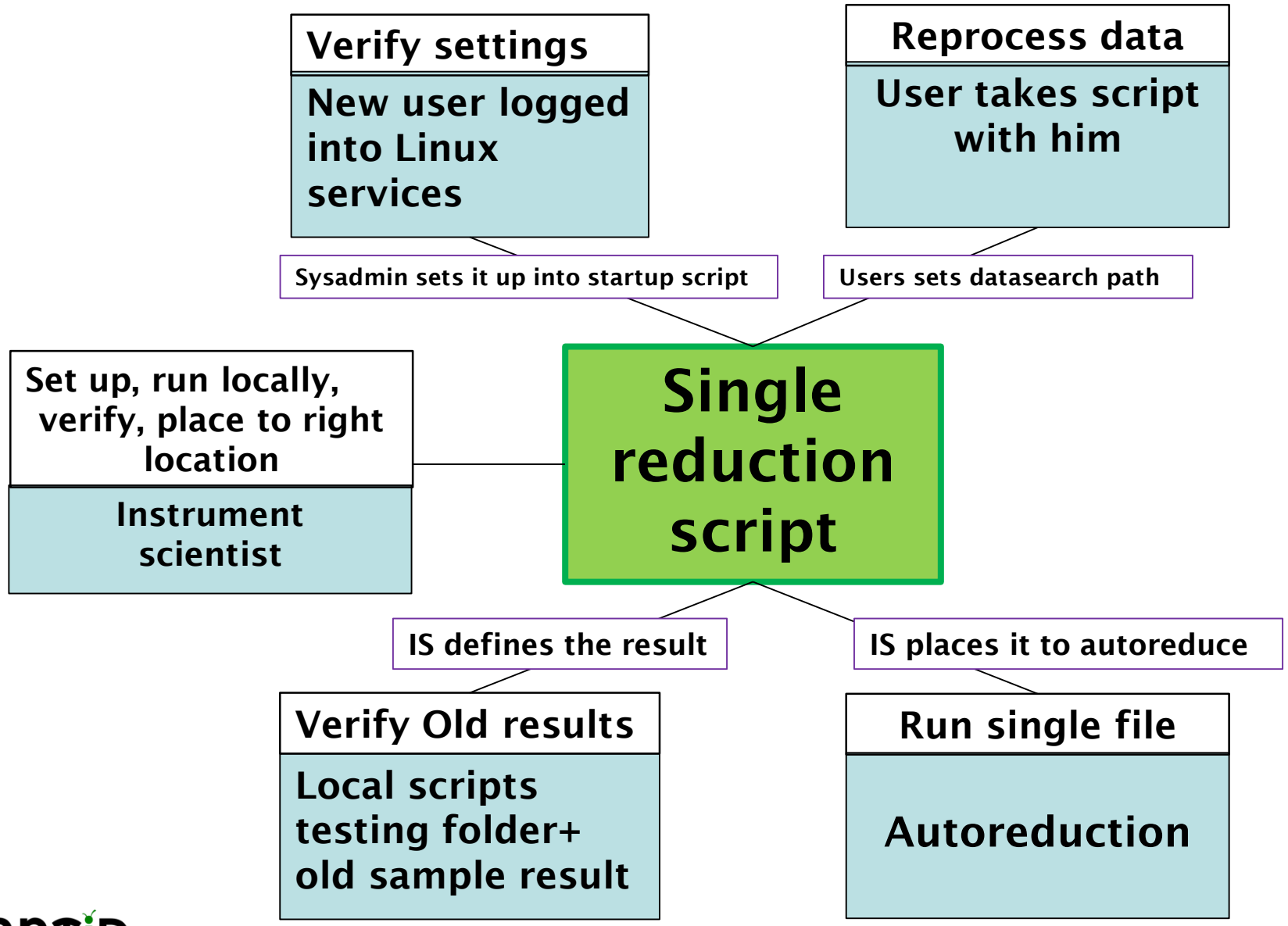
Direct Inelastic

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 progres)*

Next Release

Release v3.4

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

Thank you