IN16B Reduction

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Mantid Meeting, ILL

Outline

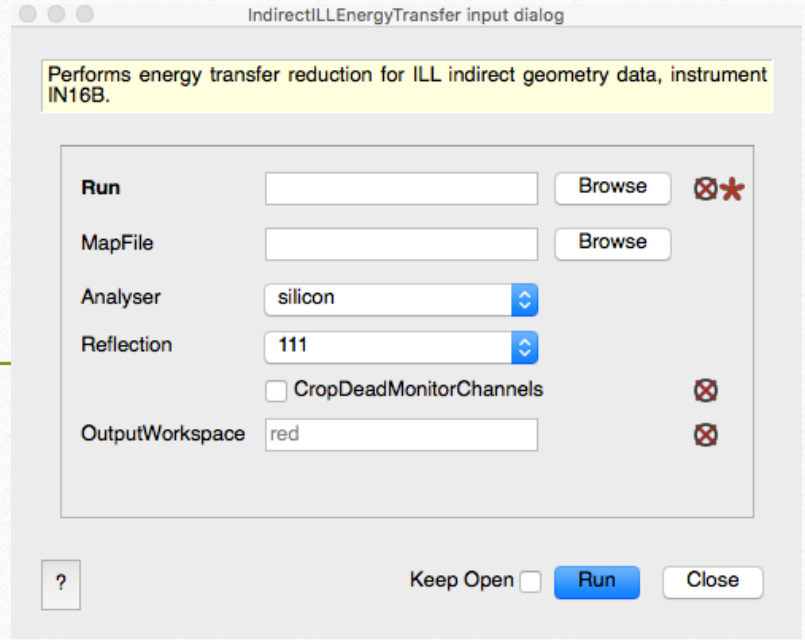
- Design and implementation
- Features and GUIs
- Validation against Lamp
- Status and future work

Multi-algorithm reduction

- The idea is to separate out the common parts of QENS and FWS into a different algorithm
- At the same time, separate the single file treatment from multiple file treatment

- ✓ More intuitive and readable
- ✓ Modular, easier to maintain
- ✓ Linear flow, no recursion
- ✓ More performant and parallel

IndirectILLEnergyTransfer



- ✓ Summing of PSD pixels
- ✓ Monitor normalization
- ✓ Transformation from channel # to energy
- ✓ Transformation of spectra axis to *theta*
- ✓ Intended to treat **single file** at a time (or multiple summed)
  - ✓ Summing *in-situ* with MergeRuns ⊗ LoadILLIndirect
- ✓ **Not** intended to be used directly by the general user
- ✓ **Fully automatic**
  - ✓ Reduction type and mirror sense deduced from *.nxs* file
  - ✓ Treats all 3 types (QENS, EFWS, IFWS) both with or without mirror sense
  - ✓ Works for data from 03.2014 onwards (when the energy, mirror sense and velocity profile are defined in *.nxs* file)

IndirectILLEnergyTransfer

Properties

Name	Direction	Type	Default	Description
Run	Input	list of str lists	*Mandatory*	File path of run (s). Allowed values: ['nxs']
MapFile	Input	string		Filename of the detector grouping map file to use. If left blank the default will be used. Allowed values: ['xml']
Analyser	Input	string	silicon	Analyser crystal. Allowed values: ['silicon']
Reflection	Input	string	111	Analyser reflection. Allowed values: ['111', '311']
CropDeadMonitorChannels	Input	boolean	False	Whether or not to exclude the first and last few channels with 0 monitor count in the energy transfer formula.
OutputWorkspace	Output	WorkspaceGroup	red	Group name for the reduced workspace(s).

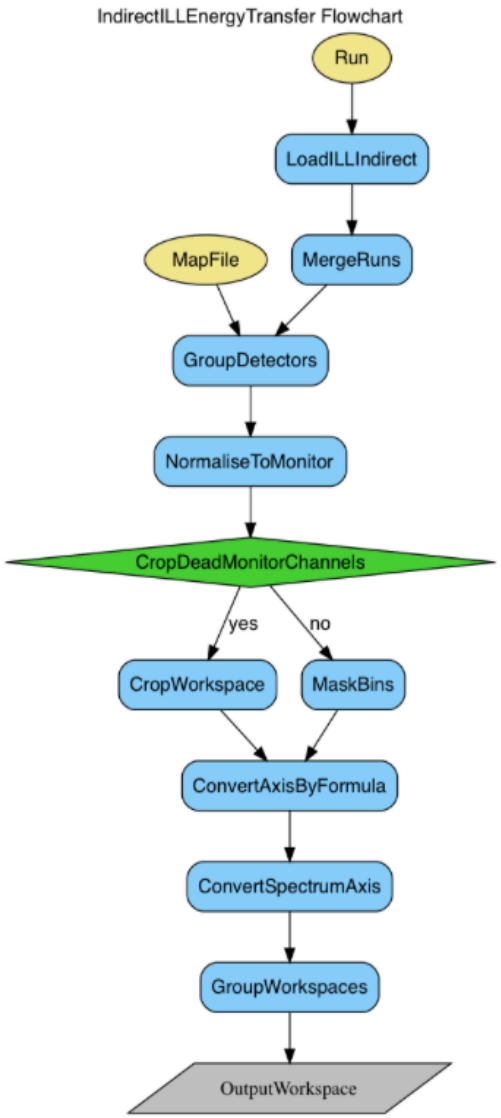
Example - IndirectILLEnergyTransfer : QENS data with mirror sense

```
ws = IndirectILLEnergyTransfer(Run='136553:136555', CropDeadMonitorChannels=True)
print "Reduced workspace has %d wings" % ws.getNumberOfEntries()
print "which have %d spectra" % ws.getItem(0).getNumberHistograms()
print "and %d bins" % ws.getItem(0).blocksize()
```

Output:

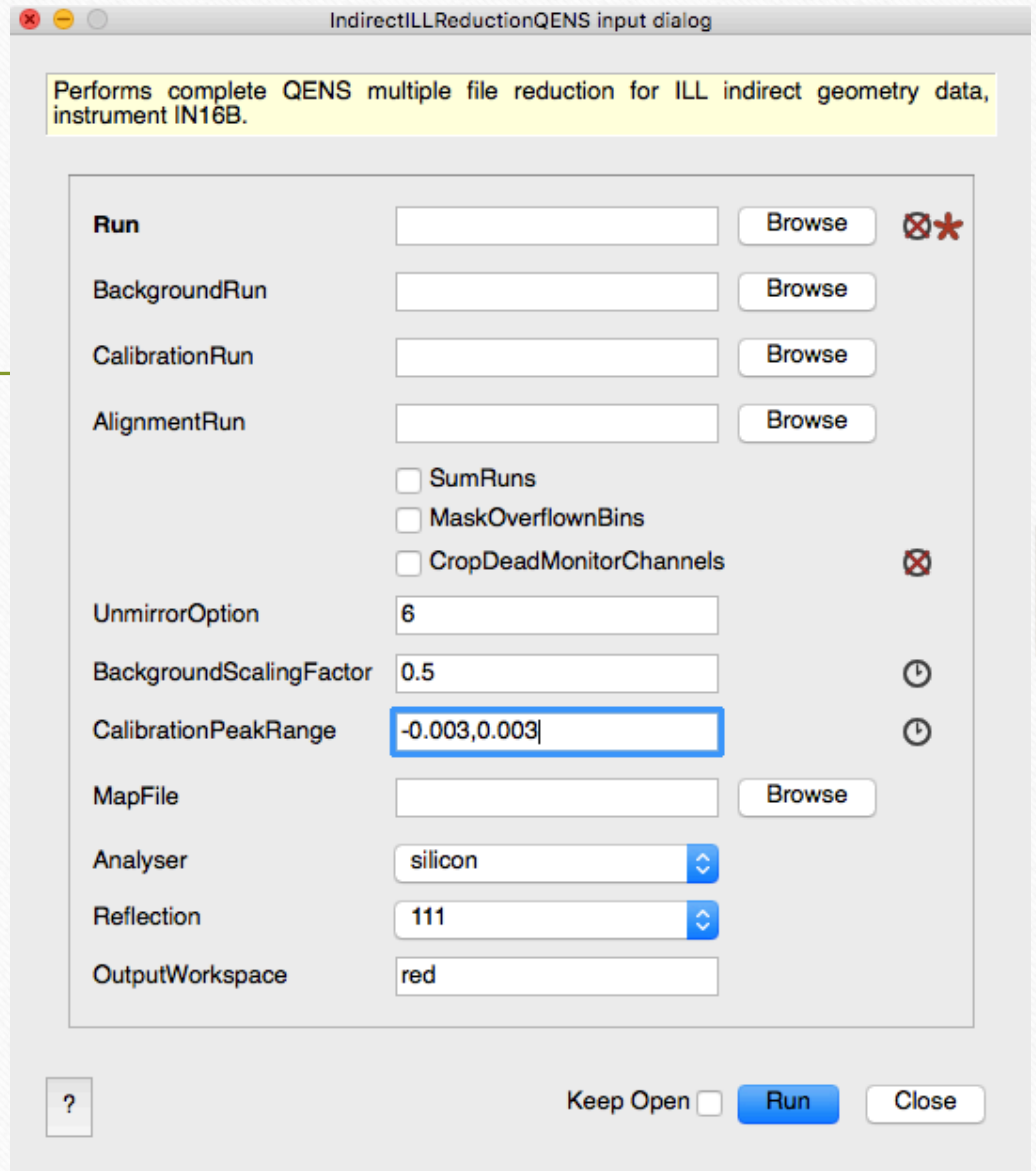
```
Reduced workspace has 2 wings
which have 18 spectra
and 1017 bins
```

Workflow



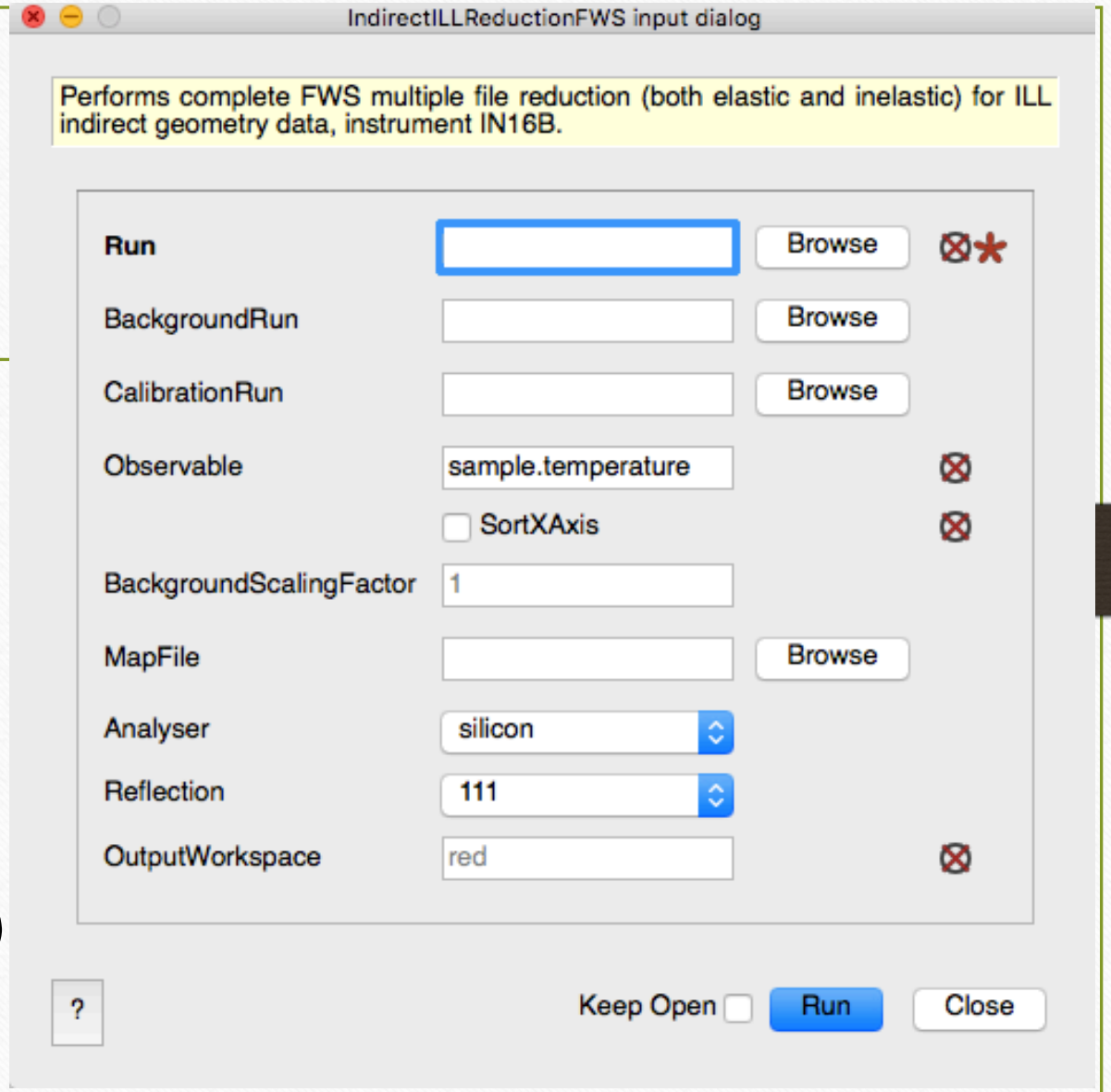
IndirectILLReductionQENS

- ✓Multiple file reduction
- ✓QENS file filtering
- ✓Background subtraction
- ✓Vanadium calibration
- ✓Unmirroring options
  - ✓0-7 for mirror sense
  - ✓0,6,7 without mirror sense



IndirectILLReductionFWS

- ✓Multiple file reduction
- ✓FWS file filtering
- ✓Background subtraction
- ✓Vanadium calibration
- ✓EFWS+IFWS in one go
  - ✓By specifying inclusive range
- ✓Integration (with automatic range)
- ✓Scan as a function of sample log

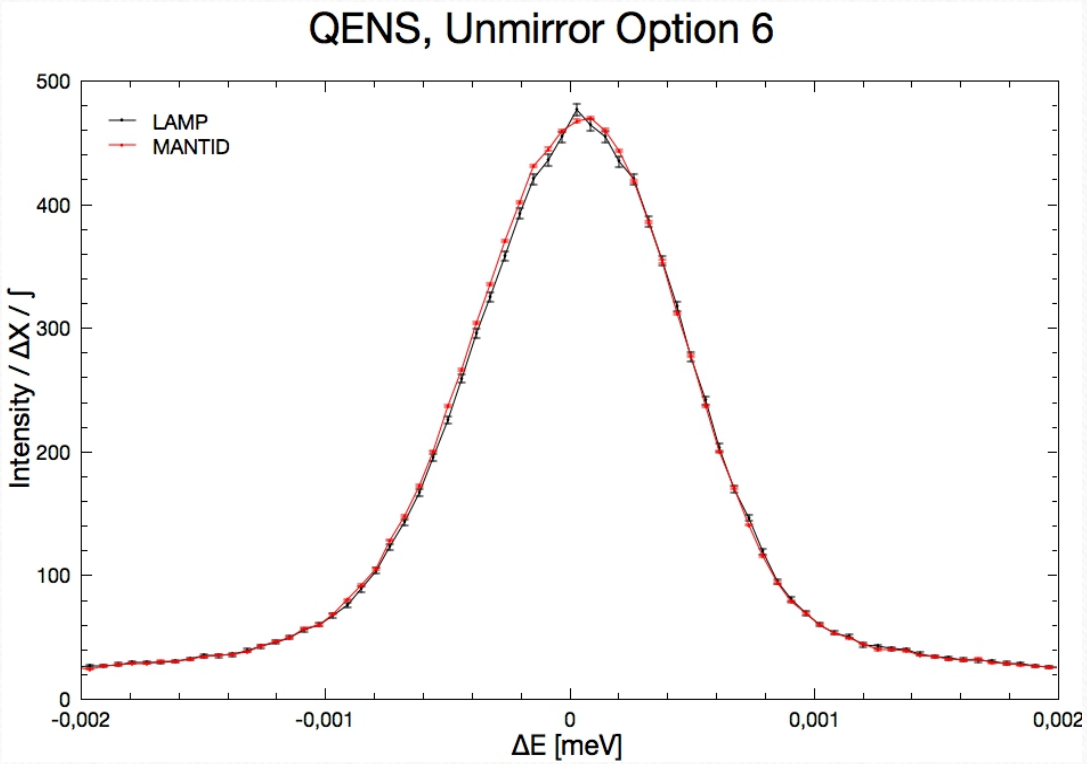


Mantid vs Lamp Comparisons

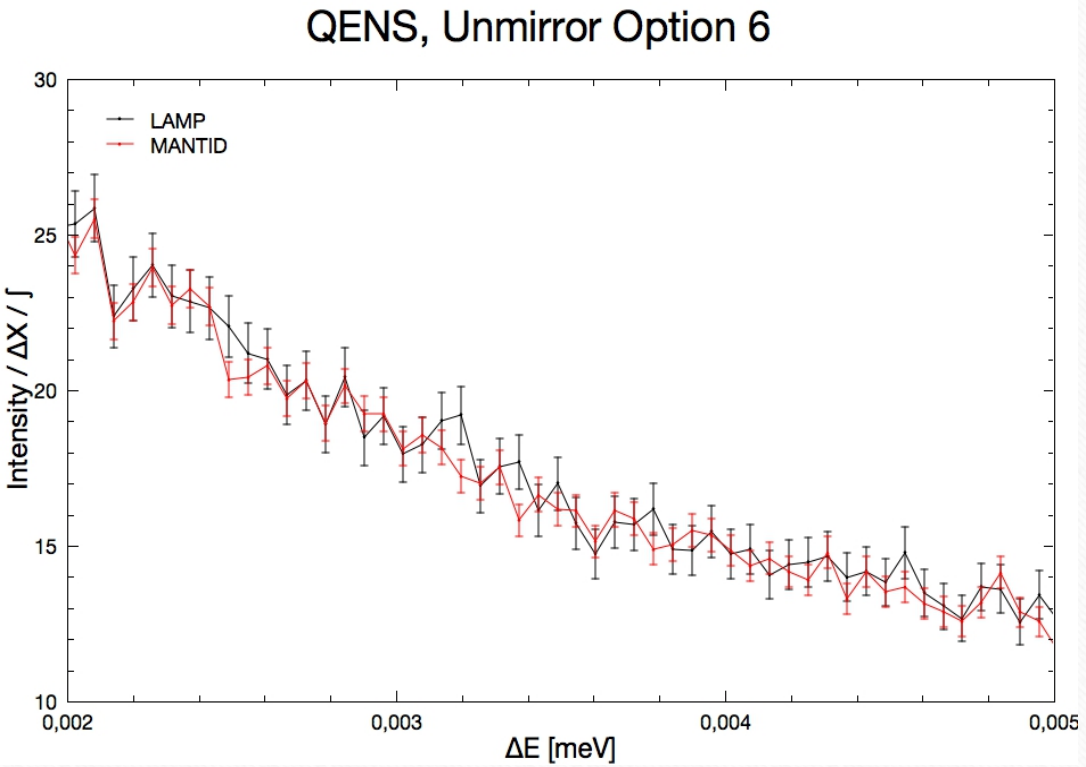
Mantid vs Lamp

- Sums over all detectors is plotted, normalized by bin width and integral
- X-axes are now identical, [-30,30] are matched to the center of the first/last bin
- No systematic shift, statistically consistent results
- Slight difference is due to peak position estimation

Center



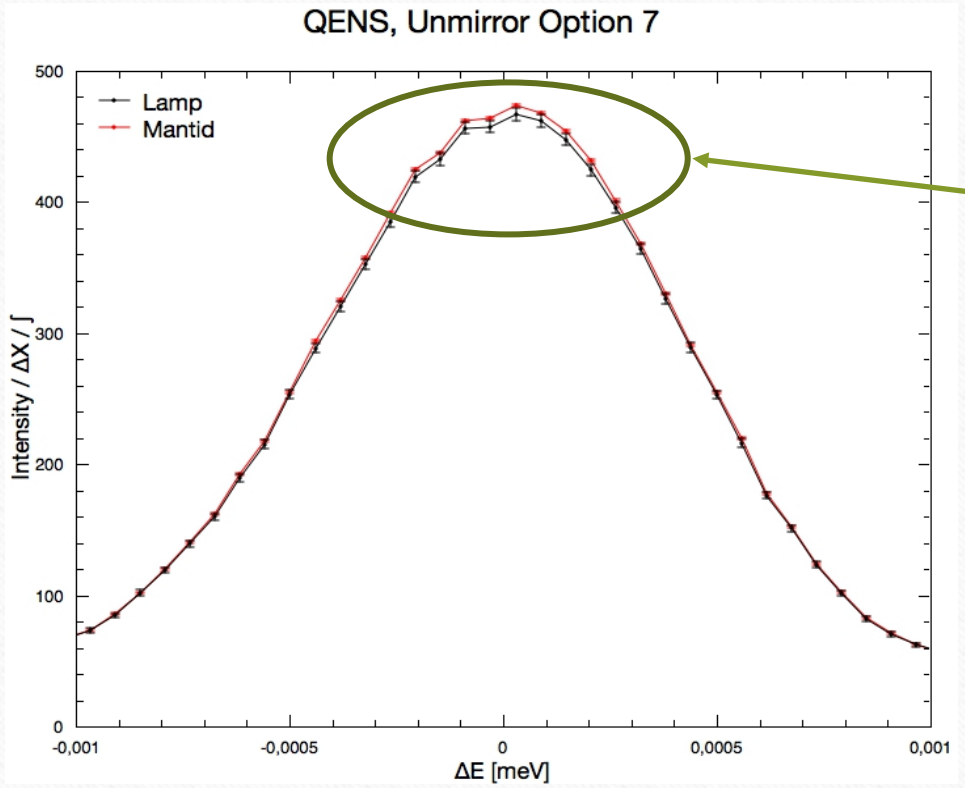
Shoulder



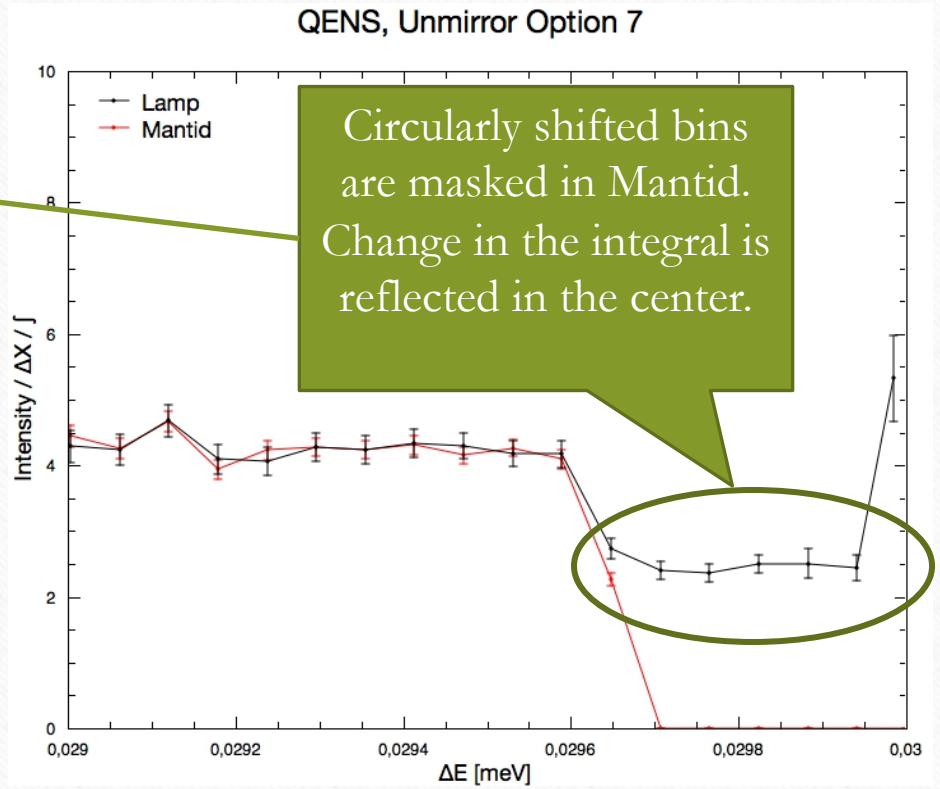
Mantid vs Lamp

- Similar results
- Note the masking

Center



Tail



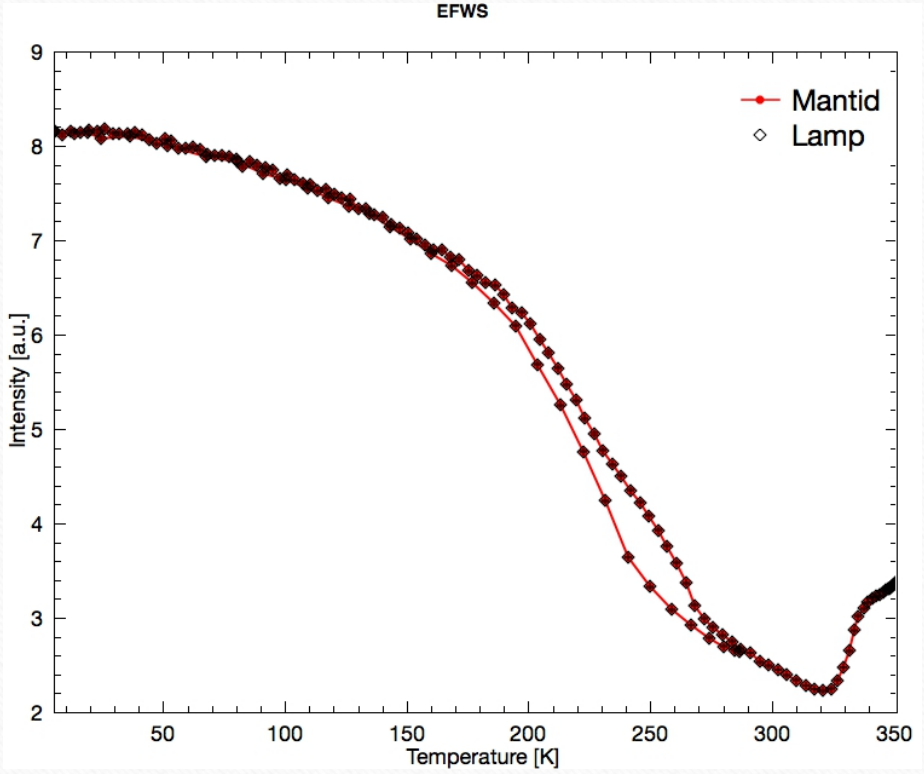
Circularly shifted bins are masked in Mantid. Change in the integral is reflected in the center.

Mantid vs Lamp

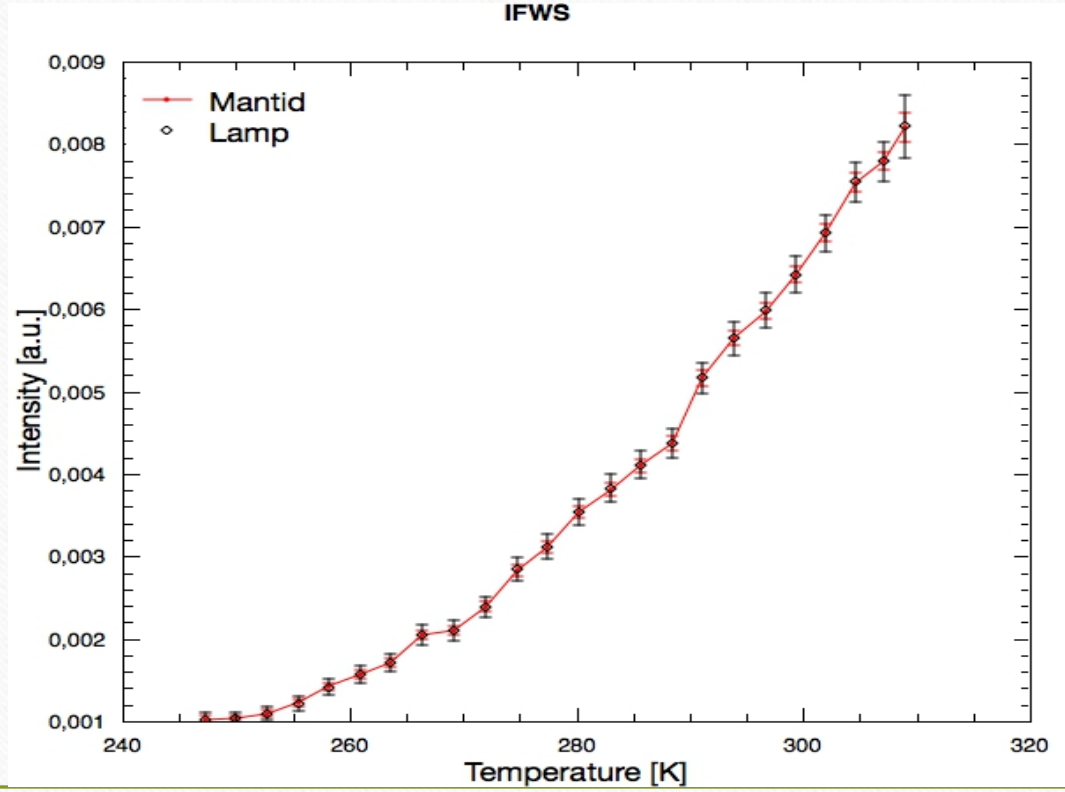
Fixed Window Scans

~identical

EFWS



IFWS



Conclusions on Mantid vs Lamp

- QENS
  - Identical shapes for unmirror 0-3, nearly identical for unmirror 4-7
  - Peak finding can lead to a couple of channel difference when the peak is not very clear
  - More often the case for noisy (less statistics) data and/or large angle detectors
  - Leading to small differences (consistent within errors) after summing the peak aligned spectra
  - Circular shifted bins in the tails are masked(zeroed) in Mantid
  - Error bars are smaller for Mantid (needs further investigation why)
  - Absolute normalization is different
- EFWS
  - Identical
- IFWS
  - Nearly identical
  - Slight difference in automatization of integration range
  - Again errors are smaller in Mantid (nearly twice)

Typical pathological case

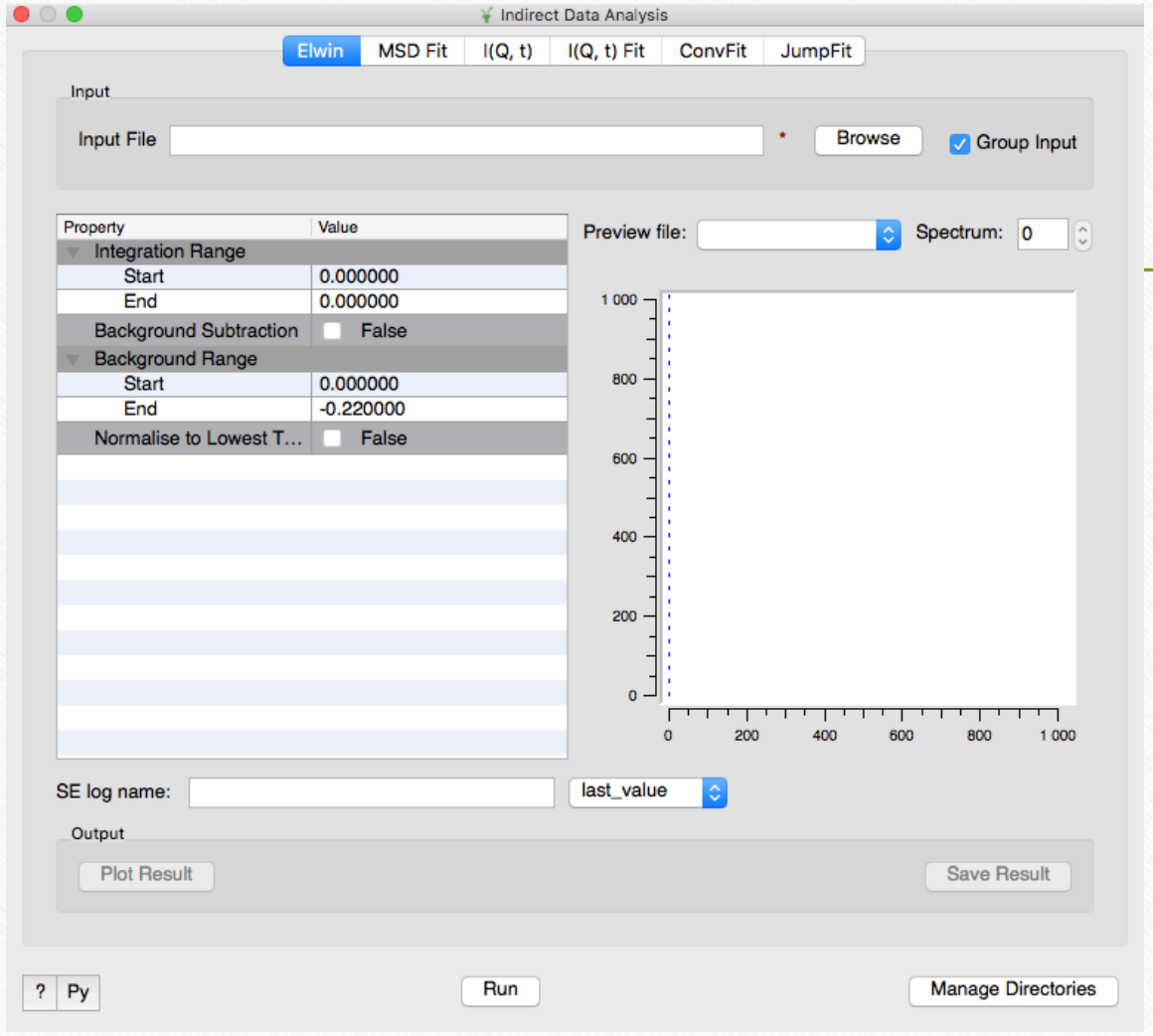
Towards this Pull Request

- ❑ Implement Sum/Interpolate options for empty can and vanadium in FWS
  - ✓ Interpolation machinery is ready (VR)
  - ✓ Happy case is straighforward, cubic splines provided by **SplineInterpolation**
  - ❖ Difficulties with corner cases (2 points, more points then in sample runs)
  - ❖ Extrapolation can only be flat
  - ❖ Note, that interpolation will work only if x-axis is sorted
- ❑ Complete 2 system tests, for QENS and FWS with updated reference histograms
- ❑ Find a nice way to convert time-stamp-like string-type sample log to a numeric value

Open points (beyond the scope of this PR)

- Moving single detectors (SD)
  - ✓ Active SDs are read from **.nxs** files
  - ❑ But their positions are still statically pre-defined in .xml IDF (moreover, not sure if all the slots are correct)
  - ❑ Right now could lead to unexpected SD angles
  - ❑ Need to search for a way how to move the detectors in the **LoadILLIndirect**
- Incorporate absorption corrections into workflow
  - ✓ Algorithms exist that compute and apply the corrections
  - ❑ Need to integrate into reduction, same task as for TOF
- Alternative (lamp-like) way of defining the PSD integration range in **IndirectILLEnergyTransfer**
  - ✓ Right now it is done with .xml grouping file, as inherited from Spencer's version
  - ✓ More powerful since one can have different integration range per each tube
  - ❑ But it is dealing with detector IDs, so one should really know what is modifying, not for a general user
- Make Indirect Analysis tools work **also** for IN16B **reduced** data

Indirect -> Data Analysis



- Elwin not needed, we do it in reduction step
  - and not only for EFWS, but also for IFWS
  - except Normalize To Lowest Temperature

- The rest is probably interesting
- (MSD, Conv, Jump Fits)
- They expect certain type of **reduced** data format
- Which is not exactly consistent between (OS)IRIS and IN16B
  - E.g. the y-axis unit, workspace grouping, etc.
  - We do a lot more in reduction step
- Need to make the analysis workflows/GUI accept also our format if IN16B is chosen as instrument
- Needs further investigation on what is actually executed behind the GUI