Indirect Corrections/Analysis in Mantid

12.12.16, Bastille weekly

Gagik

From reduction to analysis

- Separate interfaces (and underlying algorithms) exist in Mantid for ISIS indirect geometry data treatment following the reduction
- There are few differences between IN16B reduced and (OS)IRIS reduced data, preventing the use of these
- The goal was to make these compatible as much as possible with minimum intervention to analysis/corrections routines and interfaces

User experience in (OS)IRIS

- The full data treatment is run in multiple steps in different GUI interfaces
  - Typically, there is one algorithm behind each interface tab, and few tabs in each interface window
  - These mostly follow the **left-to-right** intuitive order (with few exceptions)
  - (of course one can have a python script that calls all the steps in sequence)
- Reduction interface tab itself does the energy transfer conversion
- Separate interface tab exists for performing vanadium calibration
- Another interface window for container subtraction
  - (with or without paalman & pings corrections)
- And many algorithms for different analyses live in different tabs in analysis window
- I/O between the steps is controlled by simple suffixes of the workspace/file names
  - E.g. **_raw**, **_red**, **_res**, **_calib**, **_sqw**, **_iqt**, **_eq2**, **_result**, etc.

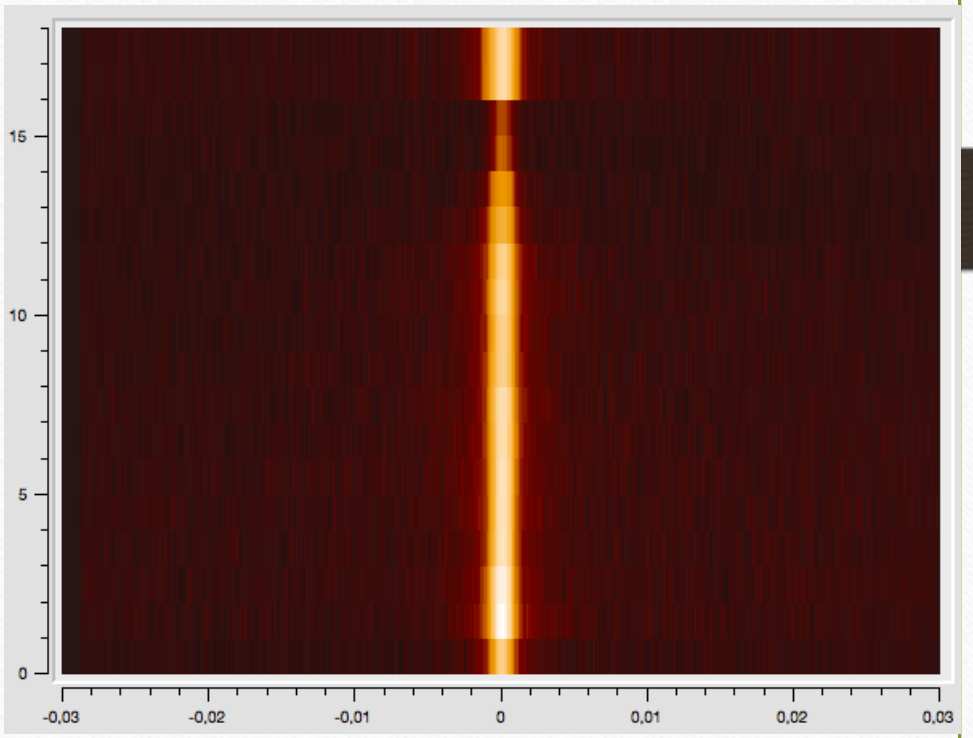
Reduced data formats

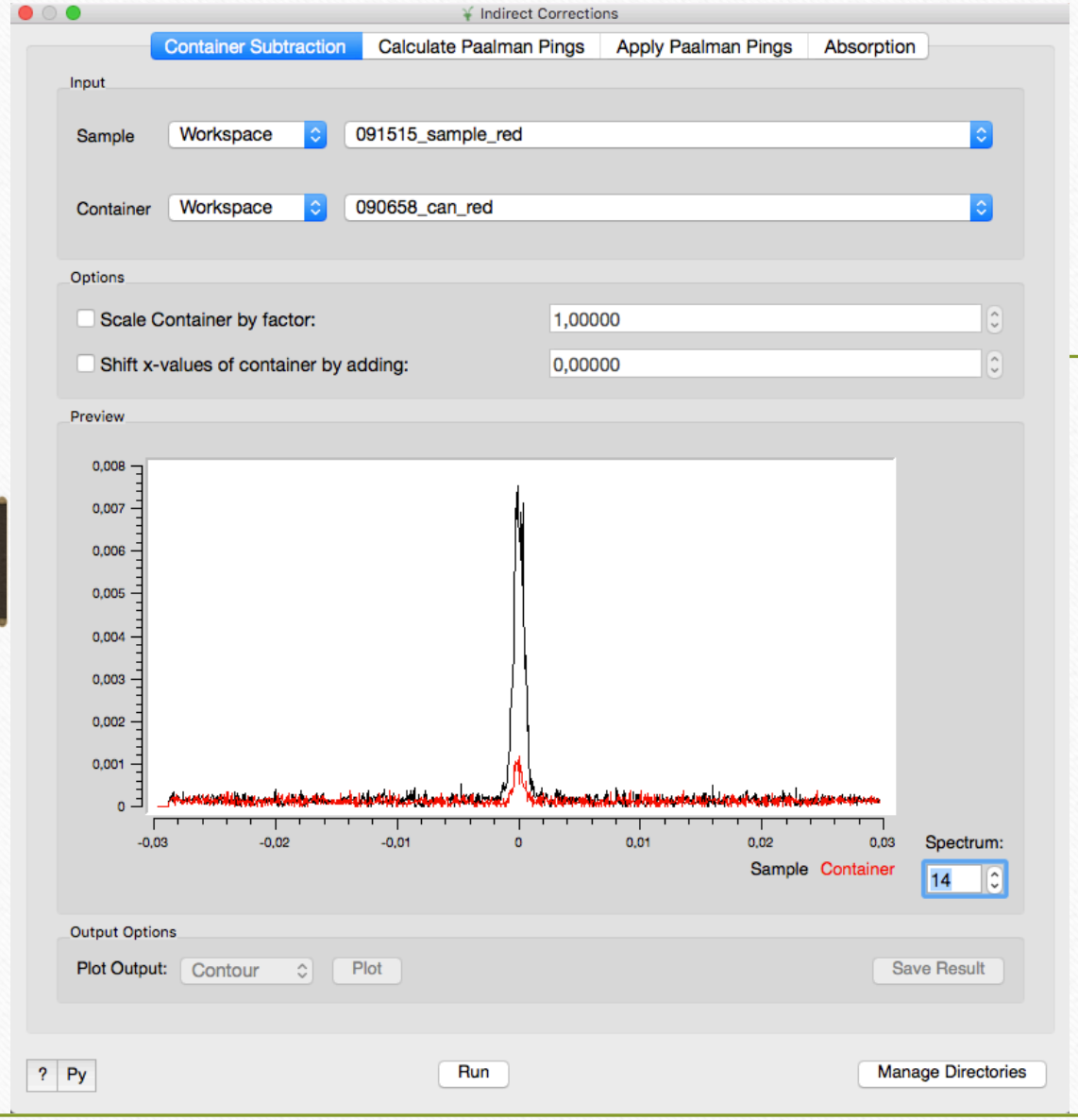
IRIS	IN16B
✓ Energy transfer as x-axis in *mev*	✓ Energy transfer as x-axis in *mev*
❑ Raw spectrum number as y-axis	❑ 2theta as y-axis
❑ **_red** suffix in workspace/filename	❑ No suffix
❑ Single workspace	❑ Workspace group*
❑ Separate reduced sample and can	❑ On-the-fly can subtraction*

Complying to the standards here is enough to make the most of the tools work out of the box.
Is there any objection against these?

Y-axis

- If left as raw spectrum number, single detectors will appear on the top
- The loader loads the multi-detectors first
- Since the number of single detectors can (in principle) be different
- So it will look different from LAMP
- One can of course convert to any unit (2theta, Q, Q^2) with one call to **ConvertSpectrumAxis** algorithm





Indirect -> Corrections GUI

- For computing and applying absorption/paalman & pings corrections
- Nice tool integrated for visualizing the sample, can, and subtracted spectra
- ✓ Everything seems to work, if the mentioned conventions are met

Resolution file for needed for analysis

- **_res** file/workspace is simply the reduced vanadium with summed spectra
- Is produced in calibration tab in reduction GUI
- Will discuss this on Wed with Louise, Spencer