

Backscattering (IN16B) reduction

Feedback from Miguel

09.03.17

Multifile limit

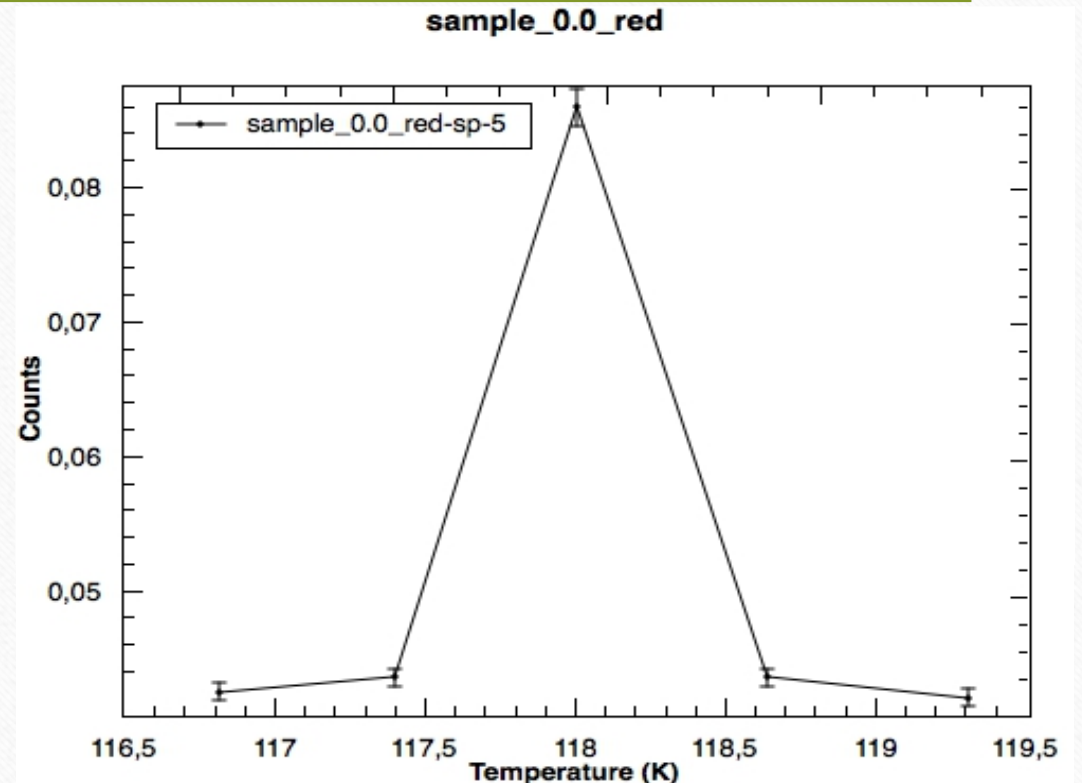
- **Multiple file loading limit – 100 is not enough for Fixed Window Scans**
 - Now made facility dependent through `Facilities.xml`
 - It is defined 1000 for ILL, and 100, as before, for other facilities
 - Still the setting can be overridden by the user via config service
 - `config['loading.multifilelimit'] = '555'` (for the current session)
 - Then `config.save()` to remember the setting
 - Or modifying the entry in `Mantid.user.properties`

Input validation in MatchPeaks

- When giving incompatible vanadium run for unmirroring (different number of energy channels) an unhandled numpy error was occurring
 - Fixed in **MatchPeaks::validateInputs** (Verena)
 - It is now handled properly and will throw a more instructive error message

mirror_sense in EFWS

- When mirror sense is ON, the data is organized in two "wings"; left and right, for doppler acceleration and deceleration phases
- For Elastic Scan, however, the doppler is OFF, so mirror sense is ambiguous
- Currently the logic is, if the mirror sense is ON, each wing is treated individually, and then they are summed
- Example dataset 140678–140682 is EFWS with mirror sense
- It turns out that for 140680, the data and monitor counts are indeed split to elastic channels of left and right wings, but for the other numors, only the left wing is actually populated
- This generates a factor of 2 (approx.) during the monitor normalization step
- $\frac{N_L}{M_L} + \frac{N_R}{M_R} \neq \frac{N_L + N_R}{M_L + M_R}$



General remarks

- When changing the normalization option from histogram to distribution or other way around, it would be good that the y-axis is scaled automatically.
 - Happens in `Graph.cpp` of `MantidPlot`, uses `QwtPlot`
 - Issue created, under investigation, lower priority
- Need to think of a way to give easy access to new users to relevant instrument documentation (docs, help, scripts, tutorials)
 - Suggestions?

New features to add

- Convert spectrum axis to Q option
- Possibility to subtract empty container also from vanadium, can be the same as for the sample, or different
- Automatic QENS data reduction? Just give full list and decide automatically which runs go together using a given parameter and tolerance (e.g. Temperature)
 - Seems the best is to group at the very beginning at raw level, i.e. right after loading
 - Normalization safety (sum/average)
 - Performance; the reduction will need to run for fewer workspaces, if they are grouped initially
 - A new general purpose algorithm, e.g. GroupBySampleLog ?

CalculatePaalmanPings

- ✓ Now you can compute also for Fixed Window Scans
- ❖ Some refactoring work in progress by Spencer & Co.
- ❑ Need to implement the interpolation of the container workspace to sample in **ApplyPaalmanPings** for point data

The screenshot shows the 'CalculatePaalmanPings' software interface. The title bar indicates 'Indirect Corrections'. The main window has four tabs: 'Container Subtraction', 'Calculate Paalman Pings' (selected), 'Apply Paalman Pings', and 'Absorption'.

Input Section:

- Sample: File [dropdown] [text field] [Browse]
- ☐ Use Can: File [dropdown] [text field] [Browse]

Correction Details Section (highlighted with a red box):

- Emode: Indirect [dropdown]
- Efixed: 0,00 meV [text field]
- Number Wavelengths: 10 [text field]
- ☒ Interpolate

Shape Details Section:

- Sample Shape: Flat Plate [dropdown]
- Sample Inner Radius: 0,000 cm [text field]
- Sample Outer Radius: 0,000 cm [text field]
- Container Outer Radius: 0,000 cm [text field]
- Beam Height: 0,000 cm [text field]
- Beam Width: 0,000 cm [text field]
- Step Size: 0,0020 [text field]

Sample Details Section:

- Mass Density: 0,00 g/cm3 [text field]
- Chemical Formula: [text field]

Can Details Section:

- Mass Density: 0,00 g/cm3 [text field]
- Chemical Formula: [text field]

Output Options Section:

- Plot Output: Wavelength [dropdown] [Plot]
- [Save Result]

Footer:

- [?] [Py]
- [Run]
- [Manage Directories]