Notes from TOF/BS discussion

April 2nd 2015 @ 14 hrs

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Objective: requirement capture and description of work for current and future TOF & BS techniques to be implemented in Mantid.

Notes from meeting/discussion and subsequent thoughts

Methods and algorithms (general)

- Methods have been described separately as linear workflows
- Algorithms (e.g. peak/background determination) have been identified as those operations that may not be available as standard operations in the Mantid framework (e.g. addition, multiplication, etc of workspaces).
- Algorithms must however be generic, as far as possible, so that they can be widely used.
- The 'devil is in the detail' - methods and algorithms must be defined in sufficient detail, indicating corresponding LAMP or other algorithms where relevant.
- A coherent set of methods can be combined in an application based on a flowchart which shows the common and distinct parts of the data treatment and defines the objects and methods of the application (see examples in PPT file)

Algorithms specific to TOF/BS

- Single crystal data should be corrected for self-shielding
- Masking detectors and not changing the data size is better than removing detectors (e.g. *remove_spectra* in LAMP) which does change the data size (Bjorn F).
- Converting S(2theta,w) to S(Q,w) and rebining at the same time (as in *sqw_rebin* in LAMP) is more efficient than doing these operations sequentially (Bjorn F).
- High resolution GaAs BS data may require an additional 'gravity' correction (TS).
- Corrections are more accurate but more time consuming if all pixels are kept through to the end of the data reduction (e.g. don't radially integrate over the detector for isotropic scattering samples). But 'collapsing' the data as soon as possible allows problems to be seen quickly (JO).
- Reducing TOF isotropic data defines the standard reduction workflow if all corrections are applied pixel-wise, as at ISIS. The time to treat data at ISIS this way is OK (Bjorn F).
- Examples of algorithms can also be found in codes like CROSSX, INX, FRIDA, etc as well as LAMP (Bjorn F).
- Multiple scattering – no working codes are available from MSCATT (John Copley), DISCUS (Harwell), Sachetti/Petrillo group (Italy), Davidowski (Argentina) and McStas (ILL). Anything in Mantid? (Bjorn F)

Quality control

- Base validity of new software on standard data sets and benchmarking against existing codes. Collect as many standard data sets as possible.
- Using a known, model S(Q,w), generate a data set which should be reduced so as to recover the

same S(Q,w) (Bela F)

Mantid

- For single crystal data sets, Matlab is better for slicing data than Paraview in Vates/Mantid (JO).
- Coexistence with LAMP: the purpose of Endurance/Bastille is to adapt Mantid for use at ILL and deploy it here. During the 'adaptation' phase, CS will continue to develop LAMP. Once Mantid performs as well as existing software at ILL (e.g. LAMP), future development effort will be concentrated on Mantid. At this point LAMP will be maintained/frozen, in particular to treat existing/old data, since it often takes several years to publish data from experiments.

Methods

- Kinetic experiments have been performed on IN5 (e.g. for stroboscopic measurements) but the time to write data from the current PSD (~30s) limits applications (JO)
- Event mode data would be useful for IN5 single crystal measurements to avoid data writing time (above) when data sets for individual crystal orientations are collected and to allow data over the whole dynamic range to be built up progressively by continuously repeating complete rotations (JO).
- Event mode data may be useful for BS in order to determine the corresponding Doppler speed accurately, providing this can be measured accurately enough (TS).
- Polarised neutrons – will be implemented first on Panther. A time-dependent correction for the polarisation of the 3He cell will have to be applied to the standard data treatment.

Interaction with NoMad

- A prototype, live data analysis server exists which allows NoMad to call any 'callable' data reduction and analysis software e.g. LAMP or Mantid with a script.
- At a 'basic level', all methods therefore have to be implemented as callable scripts.
- This is a low priority for TOF (Bela F).