Notes from DIF (powder/liquid) discussion

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Objective: requirement capture and description of work for current and future 'liquid and powder' diffraction 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 (FullProf, D4 software, etc) 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 DIF

- Routines exist to collapse 2D data sets (D2b, D19, D16) into 1D for Rietveld refinement, PDF and RMC analysis e.g. straight_1d/2d in LAMP.
- Often only the equatorial-plane data is used however since the instrument resolution function can be handled analytically in this case (JRC).
- Proper handling of the 2D resolution function requires a numerical model, which could come from McStas. In this case, integrating 2D data is not necessary – or effectively becomes part of analysis (JRC).
- Absorption/self-shielding corrections depend sensitively on effective density for powders (JRC/TH). These corrections are not available for hollow cylinders in the D4 suite (GC).
- Multiple scattering – corrections performed by 'correct' code for D4 data. They are essential for liquid/glass data reduction. Similarly for PDF analysis of (semi-) crystalline systems. They are not regarded as being essential/necessary in powder diffraction when only the Bragg peaks are fitted (JRC).
- Deconvolution is being tackled for D4 as part of data reduction – likely to be most important for PDF measurements on semi-crystalline materials (GC). Generally convolution of a model function is performed during data analysis

Quality control

- Base validity of new software on standard data sets and benchmarking against existing codes e.g. LAMP. FullProf, D4 suite. Collect as many standard data sets as possible.

Mantid

- A number of codes exists which can ingest directly powder diffraction data e.g. FullProf (JRC). The purpose of making available the reduction of powder/liquid diffraction data in Mantid is to provide users with a similar framework when using different techniques at ILL (e.g. powder DIF and TOF) and even at different facilities – ILL, ISIS, SNS, PSI, FRM2, ESS. Mantid also offers a wide range of data visualisation methods (MJ).
- Need to have scripting and GUI's for data visualisation and reduction (TH). This is the case in Mantid.
- 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

- Stroboscopic measurements have been performed on D20 – data could be collected in 'event mode' (TH).
- Kinetic measurements produce a series of files unless it is a motor scan (TH). This is not consistent with kinetic measurements producing one file for SANS & reflectometry. Implementation of NeXus/HDF5 for data storage, which is being generalised, will be an opportunity to standardise data storage strategies.
- Detector calibration – D2b, D20, D4, D19 have similar strategies for detector efficiencies based on multiple scan vanadium data. There is one routine for each instrument, in LAMP for D2b, D20 and D19.
- Polarised neutrons – some measurements have been performed on D20, flipping ratios have been measured on D1b. D3 is being used for liquid/glass/pdf measurements to separate coherent and incoherent contributions.
- Texture measurements – performed on D19 by Bachir Ouladdiaf with one user group. Also done on D1b. Just produce a series of 1D data sets as a function of sample orientation or analyse directly data from a 2D detector like D19.
- D16 – visualisation is important since diffraction data is often composed of several detector positions and this data should be merged for visualisation (VC).

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.