Notes from LSS/CS discussion on SANS.

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Objective: requirement capture and description of work for current and future SANS 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 GRASP/LAMP 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)

Quality control
- Easiest to base validity of new software on standard data sets and benchmarking against existing codes. Collect as many standard data sets as possible.

Mantid
- The LOQ Instrument scientist (Anne Terry) prefers LAMP/SANS_sheet to the current SANS/ISIS GUI in Mantid (IG)
- One strength of SANS_sheet is that all data and relevant info can be seen at once, including distinction of editable (white) and non-editable (grey) cells (RS)
- ILL SANS in Mantid should/must use as much of the existing algorithms and interfaces as possible – the decision on what can be used will be taken at the start of the Mantid/SANS project (MJ).
- It is important to be able to read data and manipulate it freely/easily as in LAMP (BD)
- This is possible in Mantid which, like LAMP, uses workspaces (with names rather than numbers) and a programming language to operate on them (Python instead of IDL)
- 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 (LAMP and GRASP for SANS), future development effort will be concentrated on Mantid. At this point LAMP will be maintained, in particular to treat existing/old data, since it often takes several years to publish data from experiments.

Methods

- Kinetic experiments currently constitute less than 10% of SANS experiments (IG)
- Polarised neutron measurements on D33 – there are a few experiments per cycle, this is expected to grow (DH)
- A couple of imaging experiments have been performed on D33 using transmitted and scattered neutrons – a routine exists in GRASP to build an image from a set of data (IG).
- Something similar may exist in LAMP from X-ray work with Bernhard Hamelin (DR)
- Event mode data will concern all 3 SANS instruments - required to monitor fast, cyclic processes which are not perfectly periodic and chemical reactions with poorly defined time scales. It is proposed to trial a time binning scheme and treat like kinetic data with variable time bin widths. Then repeat/optimise time binning to give suitable changes and statistics in reduced data. Note that Mantid handles event mode data natively since all SNS data is acquired in this mode.

NeXus files

- Data for polarised neutron measurements are currently stored in separate files for each polarisation state (DH)
- It would be consistent with other instruments at ILL and easier to manipulate data in the future if data for different polarisation states but one detector position would be stored in the same file (e.g. fewer files to enter in spreadsheets and open/read) (DR)
- Rocking curve data (multiple sample orientations) could also be stored in a single file (BD)

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.
- NoMad, in the future, can be the point at which spreadsheets of measurements (and the corresponding data) are defined and then used to call the data treatment directly or saved for use with data treatment independently i.e. automatic filling of tables like SANS_sheet
- This is one way of sorting large amounts of data (sample, water, transmission, etc) during the experiment. Otherwise it would be useful to have a tool that analyses the contents of a directory and populates a spreadsheet (IG)