BASTILLE-MANTID DIF (POWDER/LIQUID) DISCUSSION

1. Organization/steps → 1st step: requirement capture (kick-off: this meeting)

2. Scope:

Write set of workflows for each reduction-type (powder/texture, liquid/glass, strain scanning,…) :

- *Existing and future workflows*
- *Short description of algorithm/calculation for each step*
- *Does everyone agree on steps/order for a given reduction type*

Usability:

- Scripts and/or GUI
- Access from Nomad (define subset of needed commands/functionality)
- Interface: Define in detail the type of interface and functionality (starting points: LAMP & Mantid interfaces → what should be changed?)

“Quality” control:

- Set of reference measurements that can be used to cross-check?
- Benchmark with existing software (LAMP, …)
- Generate an artificial ‘perfectly known’ data set?

Determine current and future needs/types/*<u>methods</u>* of analysis:

- Powder/texture – 1D/2D (D20, D2b, D1b, D16, D19)
- Liquid/glass – (D4, D3 – new, D16)
- Strain scanning – (Salsa)
- Detector calibration
- Polarized neutrons ?
- Kinetic scans ?
- Event mode data ?
- Additional macros/tools in LAMP/IDL/Matlab/C/… ?

- D16: theta – 2 theta scan, omega scan at fixed theta (diffraction in reflection mode), background subtraction to simplify, visualise these scans

Method 1. Powder: data – 1D/2D: (2theta, h), 1D output – S(2theta)/S(Q)

1. *Read data (Ascii → NeXus) with corresponding calibration file:
   I. Sample (S),
   II. 'Background' (B)
2. Sum/join/merge (D2b, D1a, D20) data (multiple data sets)
3. Normalise to counting time or monitor counts
4. *Correct for absorption/self-shielding (S & B) – refined in TOF data, depends on packing fraction, calculated for Rietveld refinement
5. Subtract 'background' (S-B) – measured background for definition, otherwise just fitted during refinement, subtraction useful for visualisation to see small details e.g during temperature dependent measurements, correcting for lattice parameter shifts (magnetic samples, physisorption, polarised neutrons)
6. *Integrate over whole/partial detector height (D2b 2D detector)
7. Convert S(2theta) to $S(Q_{elastic})$: $Q = 4\pi(\sin(2\theta/2)/\lambda$
8. Output to FullProf, Gsas, Maud, …

* Indicates algorithms which are not standard workspace operations and are described later

Method 2. Liquid/glass diffraction: data – 1D: (2theta), 1D output – S(Q), g(r)

'Simple' from LAMP

1. *Read data (Ascii → NeXus) with corresponding calibration file:
    I. Sample (S),
    II. Empty cell (EC)
    III. Instrument background (IB)
    IV. Cadmium
    V. Vanadium for normalisation to barns (per experiment)
2. Sum & merge data (multiple data sets)
3. Normalise to counting time or **monitor** counts
4. *Correct for absorption/self-shielding (S & B)
5. Convert S(2theta) to S(Q) : $Q = 4\pi(\sin(2\theta/2)/\lambda$
6. Subtract 'background' (S-B) – linear combinations of I-V (all need to be corrected, inc 4)
7. *Apply inelastic correction
8. *Multiple scattering correction – analytical approximation (constant value for elastic, isotropic scattering), 'correct' program does inelastic, abs, multiple scattering, should do the same for powders in PDF
9. Normalisation with vanadium (treated as above) – divide sample by vanadium, could repeat backgrounds for vanadium
10. *Calculate Q(S(Q)-1)
11. Correct for resolution function – deconvolution!?!?! Benchmarking to quantify these effects, important for ordered samples, less so for liquids/glasses, resolution function known
12. *Apply window function
13. *Fourier transform data → G(r), g(r), D(r),…
14. Output for analysis codes e.g. RMC, EPSR, PDFGUI, etc

Method 3. Strain scanning

Comments:

Measuring one peak many times, link between sample and instrument coordinates

Often near 90 degrees, Debye-Scherrer cone is close to straight in this case

Fitting in LAMP OK/good (including background)

Applied stress measurements require kinetic mode (event mode data)? In-situ casting experiments can have unknown timescales hence need kinetic or event mode data.

Method 4. Detector calibration

Comment:

Calibrate for position (angle) variation of detector ‘tubes’, active zones of detectors and detector efficiency

D2b:

Angle calibration based on standard CeO_2 (?) data –performed when detector was new, but not repeated

- *Calculate average peak positions from many data sets & determine detector tube shifts so that individual data sets give peak positions that match average peak positions – see ‘calib_ang_tubes_gauss.pro’ in LAMP*

Detector active zone determination – performed each cycle (D2b detector is ‘stable’)

- *Electronic readout of detector tubes has ‘dead’ zones. Find edges of active zones and ‘map’ onto physical detector height – see ‘calib_zone.pro’ in LAMP*

Detector efficiency correction based on vanadium data – performed each cycle (D2b detector is ‘stable’)

- *Calculate average intensity from many (~20) data sets & determine height-resolved detector tube efficiencies so that individual data sets give intensities that match average intensities – see ‘calib_eff_2d_bms.pro’ in LAMP*

D19:

Vertical and horizontal electronic corrections via 2 matrices provided by the detector group

Method 4. Detector calibration

Comment:
Calibrate for position (angle) variation of detector ‘tubes’, active zones of detectors and detector efficiency

D20:
Wavelength dependent correction, sometimes used
Vanadium scans for detector efficiency – routine in LAMP

D4:
Similar to D20, D2b

Salsa:
New 3He wire detector – could be treated like e.g. D2b (2D)

D1b:
In NoMad, based on a single vanadium measurement

D16:
Based on water data – OK for long wavelength neutrons

Method 5. Polarised neutrons ?

Comments:

Treat the data as before then post-treat

But 3He cells used and need to correct for time-dependence of polarisation

Some measurements on D20, flipping ratio measurements on D1b

Depolarisation of beam by sample has to be taken into account

Method 6. Kinetic mode

Comments:

Used on high count rate instruments (D20) to e.g. follow a chemical reaction

Normally the time-dependent data is stored in a series of files (on D20), only motor scans currently put many data sets into one file.

Treating the data amounts to looping over the ‘standard’ data reduction in the preceding methods

Method 7. Event mode data – events rather than histograms in Q, time, etc

Comments:

Makes sense, in terms of file size, to use this mode when highly pixelated detector (e.g. IN5) has many zeros (background signal must be low) – not the case on a powder diffractometer at ILL?

Also when sampling almost periodic modulation of data – this corresponds to the ‘stroboscopic method’ on D20.

ALGORITHMS for POWDER DIF other than normal workspace operations in Mantid (add, subtract, multiply, etc)

To complete with references, equations, existing algorithms, etc

1.4 *Correct for absorption/self-shielding (S & B)

???

1.6 *Integrate over whole/partial detector height (D2b 2D detector)

'Straighten' Debye-Scherrer cones transforming I(2theta, h) into I(2theta_equatorial, h) or I(Q_equatorial, h) see e.g. 'straight_2d' in LAMP. Then integrate part (a simple 'total' in LAMP) or all ('straight_1D' in LAMP) of the 2D data set to produce a 1D data set.

ALGORITHMS for LIQUID DIF other than normal workspace operations in Mantid (add, subtract, multiply, etc)

To complete with references, equations, existing algorithms, etc (esp. from Henry's software)

(see prox file in LAMP)

1.4 *Correct for absorption/self-shielding (S & B)

???

1.7 *Inelastic correction

Fit parabola to high Q data and divide the data by the fit (uses STR_FIT in LAMP)

1.8 *Calculate Q(S(Q)-1)

Simple workspace manipulation, performed in d4_QSQ1 in LAMP

1.9 *Apply window function

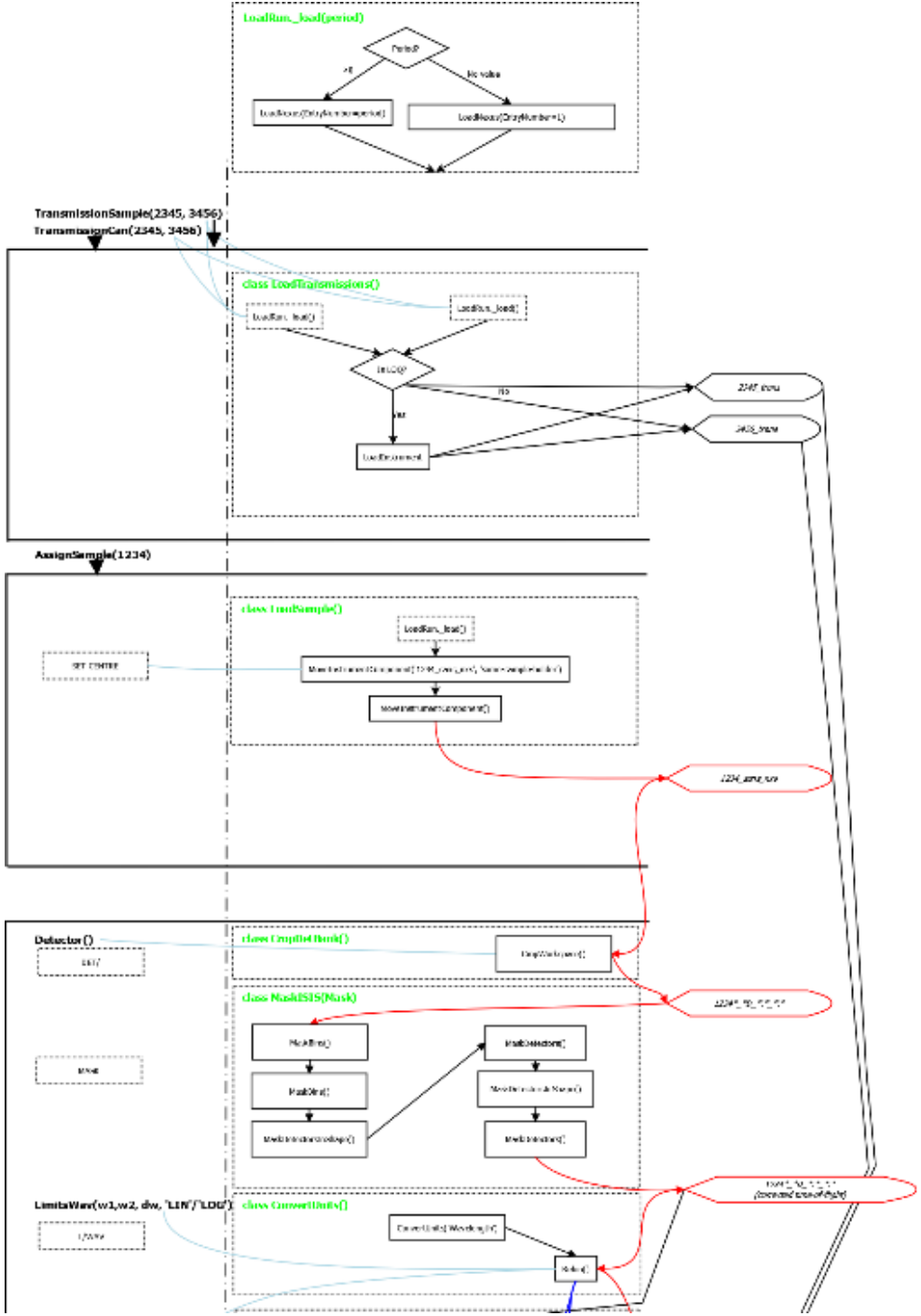
Simple workspace manipulation e.g. multiply by a sinusoidal envelope

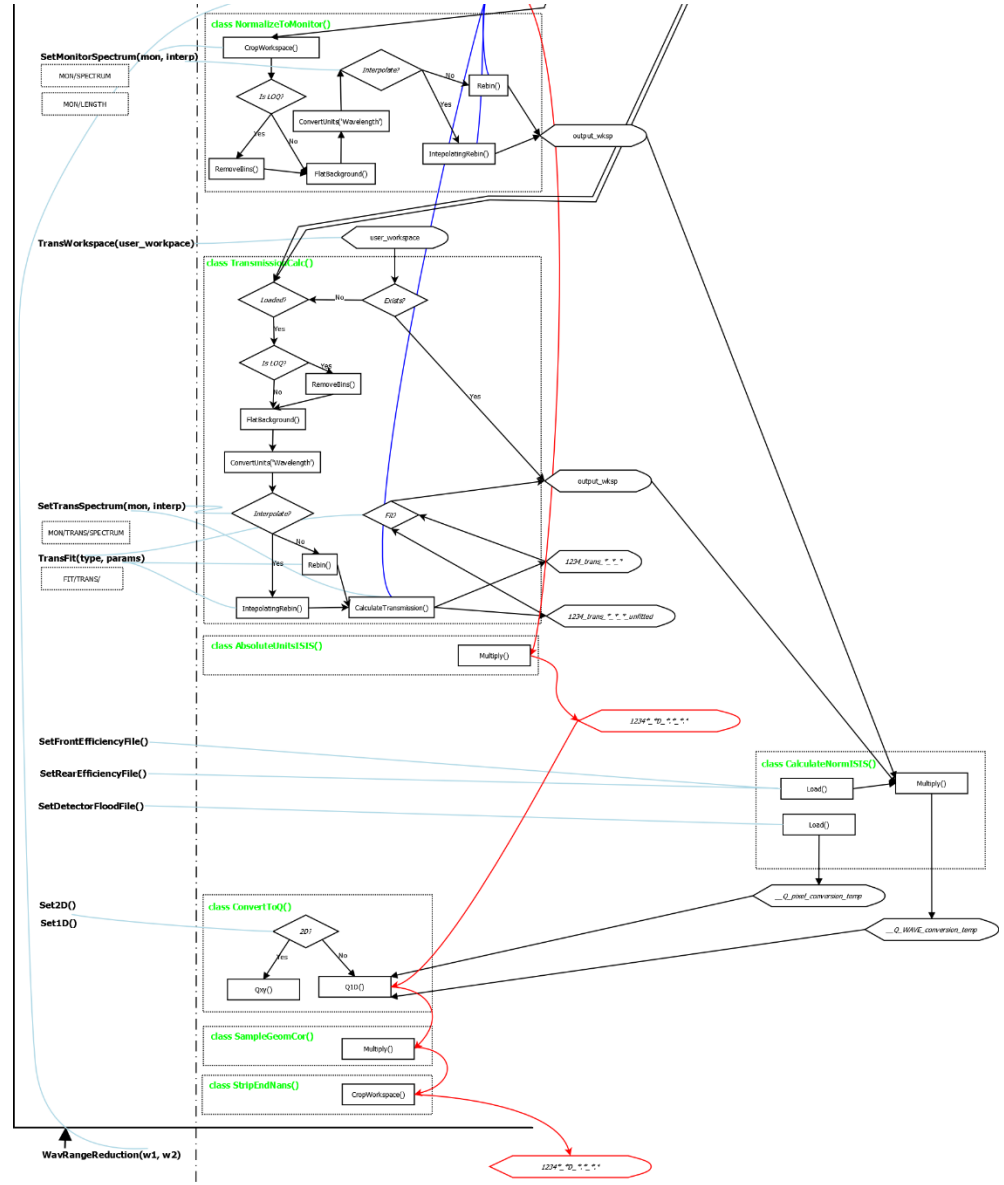
1.10 * Fourier transform data

See e.g. d4_FFT.pro

Document/details (possibly with flowcharts) to be completed by Thomas (and DIF and CS if necessary) in one month (~ June 18th 2015)

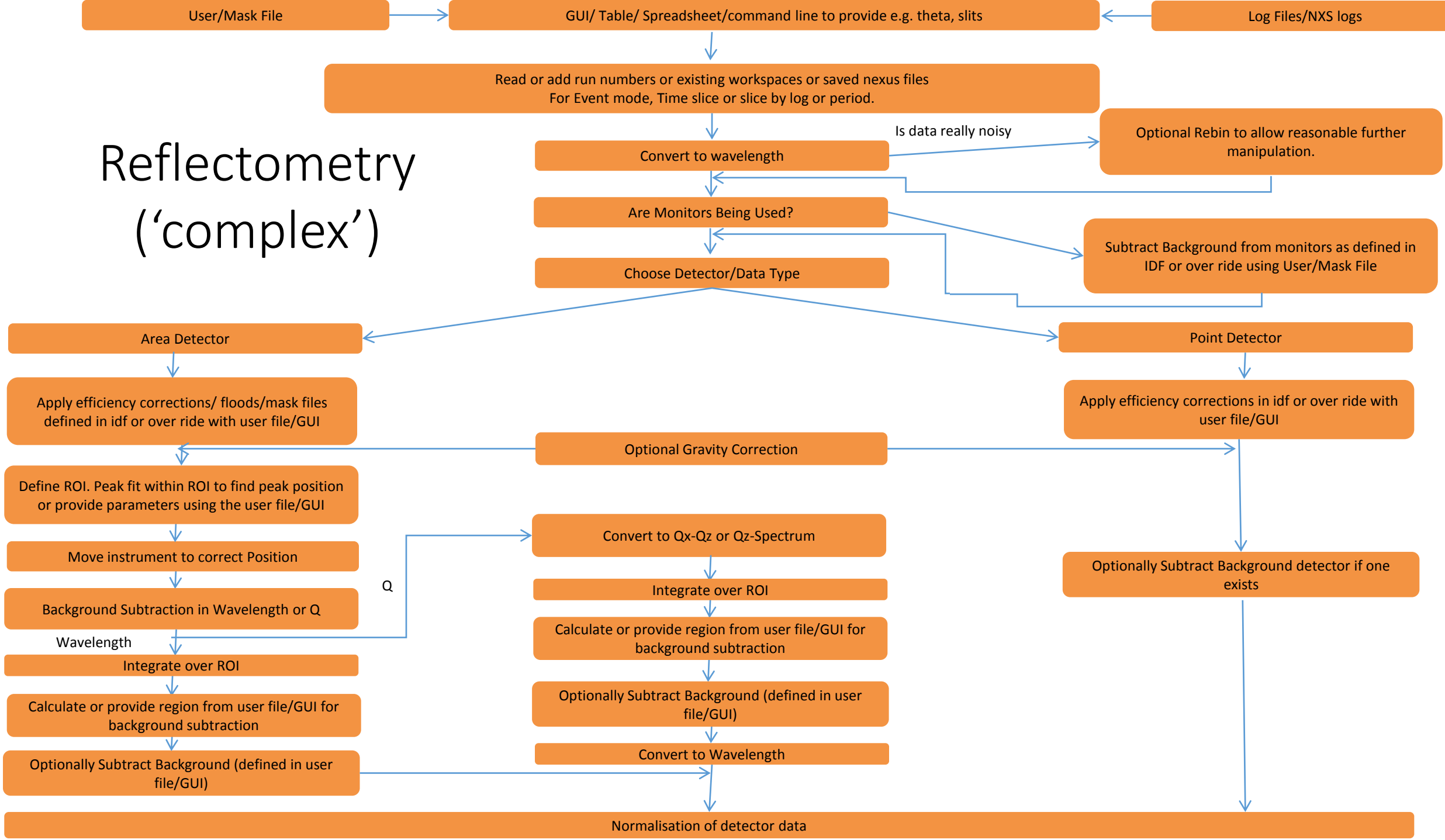
The following flowcharts show an appropriate level of detail and how different methods can be combined in a single application or GUI

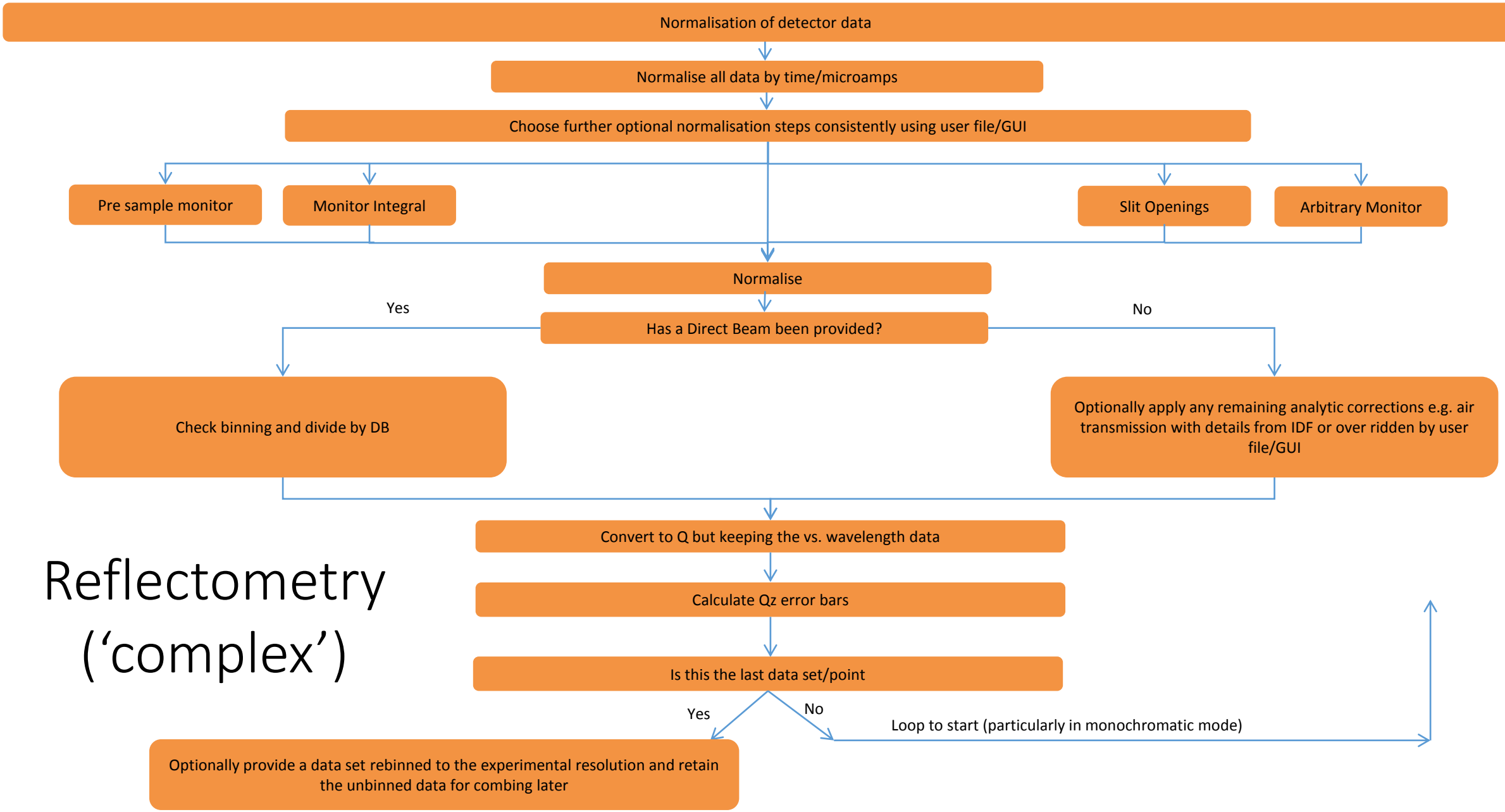




http://www.mantidproject.org/images/8/8f/ISIS_SANS_reduction.png

Reflectometry ('complex')





Reflectometry ('complex')

→ CLEAR, COMPLETE REQUIREMENT DOCUMENT