BASTILLE-MANTID TOF/BS DISCUSSION

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

2. Scope:

Write set of workflows for each reduction-type (TOF – isotropic, TOF single crystal, BS – spectrum, BS – (in)elastic scan,...) :

- *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/*methods* of analysis:

- TOF – isotropic (IN4/5/6)
- TOF – single crystal (IN5/Panther/Ramses)
- Polarized neutrons (IN5) ?
- BS – spectra (IN16)
- BS – (in)elastic scan (IN16/13)
- Kinetic scans ?
- Event mode data ?
- Additional macros/tools in LAMP/IDL/Matlab ?

Method 1. TOF – isotropic: data – 3D: (2theta, h, TOF), 2D output – S(Q,w), 1D output – GVDOS(w)

1. *Read data (NeXus):
    I. sample (S),
    II. Vanadium calibration (V),
    III. Empty vanadium (EV)
    IV. Empty cell (EC),
    V. Cadmium (Cd) – included but not cited hereafter!
2. Sum data (multiple data sets)
3. *Normalise to counting time or monitor counts
4. *Apply detector mask, remove low-counting detectors
5. *Normalise detector counts with vanadium data
6. *Correct for absorption,/self-shielding
7. *Correct for wavelength dependence of detector efficiency
8. *Convert TOF to Energy
9. *Convert S(2theta, h, TOF) to S(2theta, w)
10. *Convert S(2theta, w) to S(Q,w)
11. Rebin data to regular grid
12. *Correct for Bose factor → susceptibility
13. *Calculate generalised vibrational density of states (GVDOS)
14. *Correct multiphonon spectral contribution
15. *Correct for multiple scattering

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

Method 2. TOF – single crystal: data – 4D: (2theta, h, TOF, sample orientation), 4D output – S(Q_X, Q_Y, Q_Z, w)

Comments:

Convert 4D (2theta, h, TOF, sample orientation) data to S(Q_X, Q_Y, Q_Z, w)

Correct for absorption/self-shielding

Visualise and treat 3D volumes, 2D slices and 1D spectra

Data output from LAMP (SPE format) to HORACE today.

Integrated solution with VATES in MANTID in the future

Method 3. TOF polarised neutrons

Comments:

Will polarised neutrons be used on IN5, Panther, Ramses in the near/distant future?

Is the data treated as in methods 1 (isotropic) and 2 (single crystal) for different polarisation states and the resulting spectra are then combined?

Note: On D33 (and elsewhere) standard corrections have to take into account the (time-dependent) degree of polarisation of the incident beam.

Method 4. BS - spectra: data – 3D: (2theta, h, ‘TOF’), 2D output – S(Q_{el}, w)

1. *Read data (NeXus):
    I. sample (S),
    II. Vanadium calibration (V),
    III. Empty vanadium (EV),
    IV. Empty cell (EC),
    V. Cadmium (Cd),
2. Sum data (multiple data sets)
3. *Normalise to counting time or monitor counts
4. *Apply detector mask, remove low-counting detectors
5. *Normalise detector counts with vanadium data
6. *Correct for absorption,/self-shielding
7. *Convert ‘TOF’ to Energy
8. *Convert S(2theta, h, w) to S(2theta, w)
9. *Convert S(2theta, w) to S(Q_{el},w)
10. *Correct for multiple scattering

Method 5. BS – (in) elastic scan: data – 3D: (2theta, h, temperature-T), 2D output – I(Q_{el}, T)

1. *Read data (NeXus):
   I. sample (S) – multiple data sets to cover temperature range, 1 data set per temperature,
   II. Vanadium calibration (V),
   III. Empty cell (EC),
   IV. Cadmium (Cd),
2. *Normalise to counting time or monitor counts
3. *Apply detector mask, remove low-counting detectors
4. *Normalise detector counts with vanadium data (or sample itself at low temperature)
5. *Correct for absorption,/self-shielding
6. *Convert S(2theta, h, T) to I(2theta, T)
7. *Convert I(2theta, T) to I(Qel,T)

Note: elastic and inelastic scans may not involve continuous ranges of run numbers since the Doppler machine is stopped (elastic scan) and started (inelastic scan) for a given temperature i.e. data has to be sorted.

Method 6. Kinetic mode

Comment:

Used on high count rate instruments like SANS & reflectometry to e.g. follow a chemical reaction

Is this likely to be used for TOF and/or BS?

Normally the time-dependent data is stored in 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, TOF, 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)

Possible use for single crystal data acquisition, allowing crystal to be rotated continuously i.e. a series of angle-dependent files would be replaced by one event mode data file. This approach would remove the need to position the crystal accurately which may be relatively time-consuming

Current thinking (for SANS and reflectometry) is to inspect the event mode data 'movie', trial a time binning scheme, treat like kinetic data with variable time bin widths. Repeat/optimise time binning to give suitable changes and statistics in reduced data

ALGORITHMS for TOF other than normal workspace operations in Mantid (add, subtract, multiply, etc) complete with references, equations, existing algorithms, etc

1.1 *Read data (NeXus): data – 2D: (2theta – TOF)

1.3 *Normalise to incident beam

Divide data by counting time or monitor counts, see e.g. normalise in Lamp

1.4 *Apply detector mask

Remove spectra based on list from data set, see e.g. remove_spectra in Lamp

1.5 * Vanadium normalisation (detector calibration)

Detector efficiency corrected using vanadium spectrum (elastic intensity) see e.g. vnorm in Lamp

1.6 *Absorption/self-shielding correction

Corrections depend on sample type and geometry, see e.g. slab_tof & cylindcor in Lamp

1.7 *Correct for wavelength dependence of detector efficiency

For 3He detectors, see e.g. cor_tof in Lamp

1.8 *Convert TOF to Energy

Take into account that elastic peak may be missing or not in the same channel in every spectrum, see e.g. t2e for TOF in Lamp

1.9 *Convert S(2theta, h, TOF) to S(2theta, w)

Radial integration (over Debye Scherrer cones) for PSD (IN5 – in5_DebyeScherrer in Lamp) or simple sum (IN6 – sumbank in Lamp)

1.10 *Convert S(2theta, w) to S(Q,w) & 1.11 rebin to regular grid

See sqw_rebin, reb, estrip, qstrip, etc in Lamp

ALGORITHMS for TOF other than normal workspace operations in Mantid (add, subtract, multiply, etc) complete with references, equations, existing algorithms, etc

1.12 *Calculate susceptibility

Correct spectrum for Bose factor, see e.g. kis in Lamp

1.13 *Calculate GVDOS

Correct spectrum for Bose factor and apply q-dependent correction (incoherent approximation 'Bredov-Ostowskii') in e.g. gdos in Lamp

1.14 *Correct multiphonon contribution

See e.g. muphocor in Lamp (from Helmut, Stef also has a simpler routine?)

1.15 *Correct for multiple scattering

Done when fitting as in e.g. Discus

ALGORITHMS for BS other than normal workspace operations in Mantid (add, subtract, multiply, etc) complete with references, equations, existing algorithms, etc

4.3 *Normalise to monitor

Takes into account monitor spectrum, see e.g. bsnorm in Lamp

4.6 *Absorption/self-shielding correction

As for TOF, algorithm 1.6

4.7 *Convert 'TOF' to Energy

Takes into account monochromator speed and d-spacing, see e.g. tee in Lamp

4.8 *Convert S(2theta, h, w) to S(2theta, w)

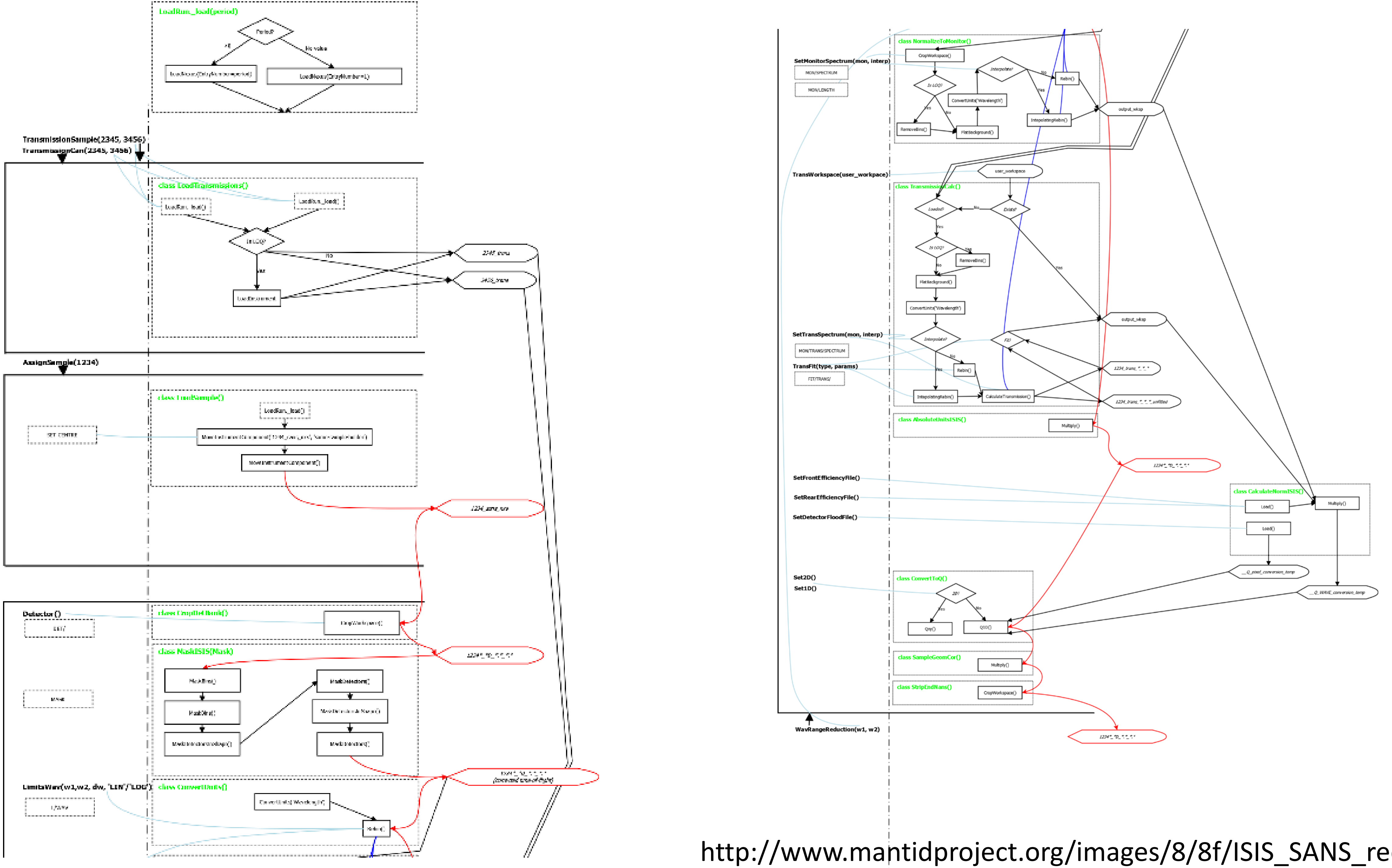
Sum over detector height of PSD

4.9 *Convert S(2theta, w) to S(Q_{el},w)

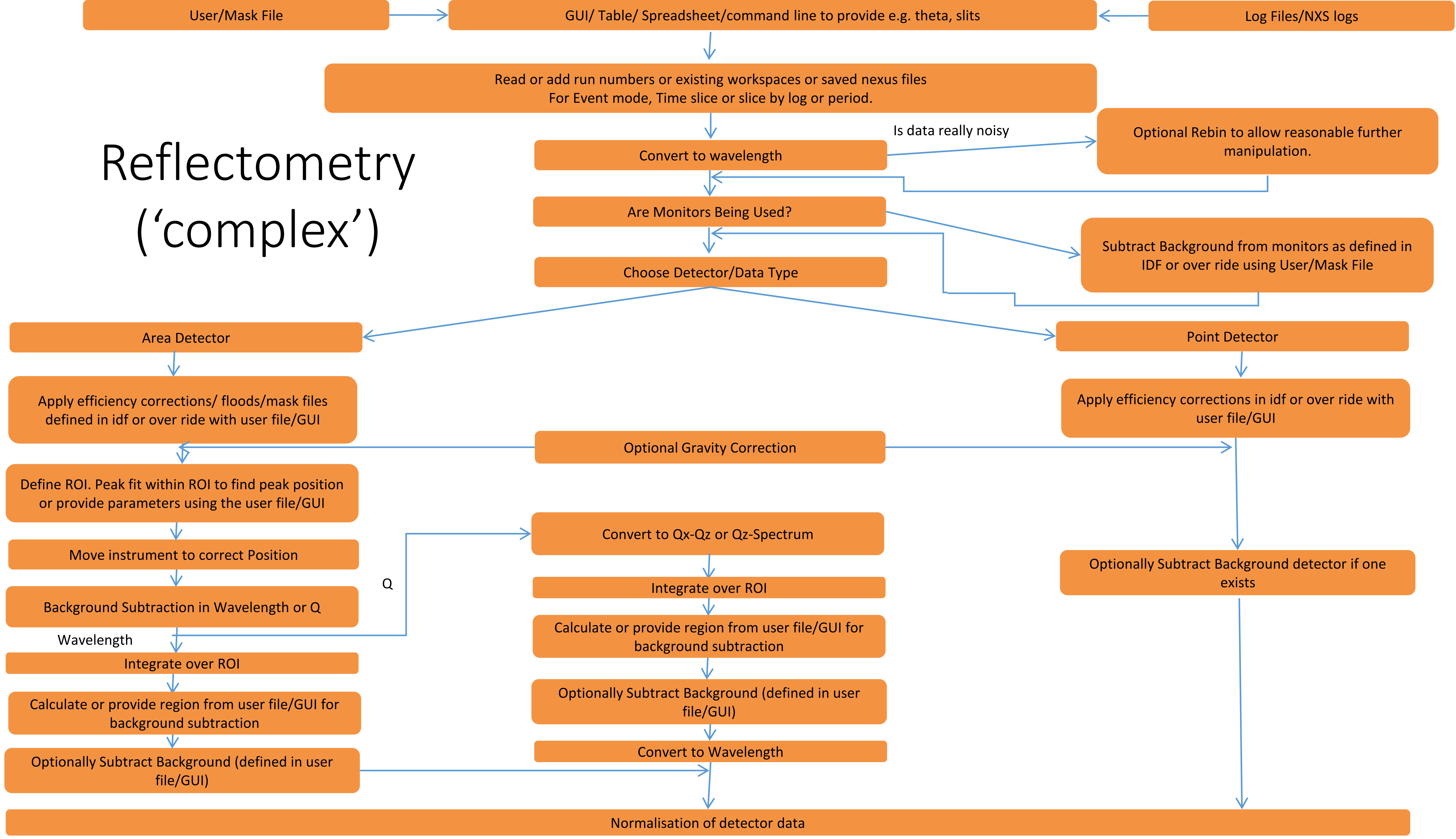
*Conversion from 2theta to Q i.e. Q=(sin (2theta)/2)*4pi/lambda*

Document/details (possibly with flowcharts) to be completed by Bjorn (and TOF and CS if necessary) in one month (~ May 2nd 2015)

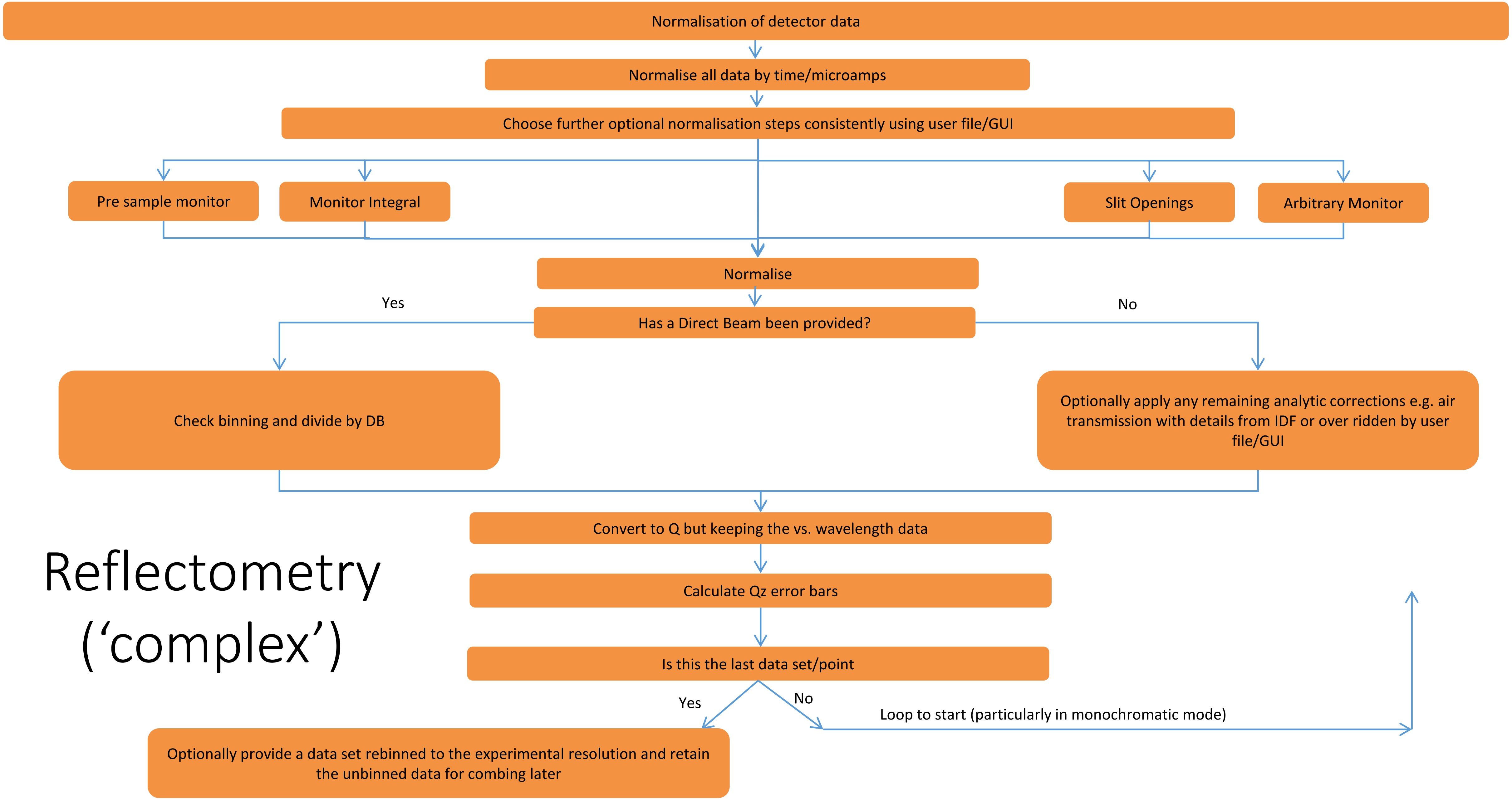
The following flowcharts show an appropriate level of detail and how different methods can be combined in a single application or GUI



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


Reflectometry
('complex')
User/Mask File
GUI/ Table/ Spreadsheet/command line to provide e.g. theta, slits
Log Files/NXS logs
Read or add run numbers or existing workspaces or saved nexus files
For Event mode, Time slice or slice by log or period.
Convert to wavelength
Is data really noisy
Optional Rebin to allow reasonable further manipulation.
Are Monitors Being Used?
Subtract Background from monitors as defined in IDF or over ride using User/Mask File
Choose Detector/Data Type
Area Detector
Point Detector
Apply efficiency corrections/ floods/mask files defined in idf or over ride with user file/GUI
Apply efficiency corrections in idf or over ride with user file/GUI
Optional Gravity Correction
Define ROI. Peak fit within ROI to find peak position or provide parameters using the user file/GUI
Move instrument to correct Position
Background Subtraction in Wavelength or Q
Q
Wavelength
Integrate over ROI
Calculate or provide region from user file/GUI for background subtraction
Optionally Subtract Background (defined in user file/GUI)
Convert to Qx-Qz or Qz-Spectrum
Integrate over ROI
Calculate or provide region from user file/GUI for background subtraction
Optionally Subtract Background (defined in user file/GUI)
Convert to Wavelength
Optionally Subtract Background detector if one exists
Normalisation of detector data

Reflectometry ('complex')



→ Clear, complete requirement document