BASTILLE-MANTID SANS DISCUSSION

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

2. Scope:

Write set of workflows for each reduction-type (classic SANS, isotropic, 2D, TOF, kinetic, polarised,…):

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

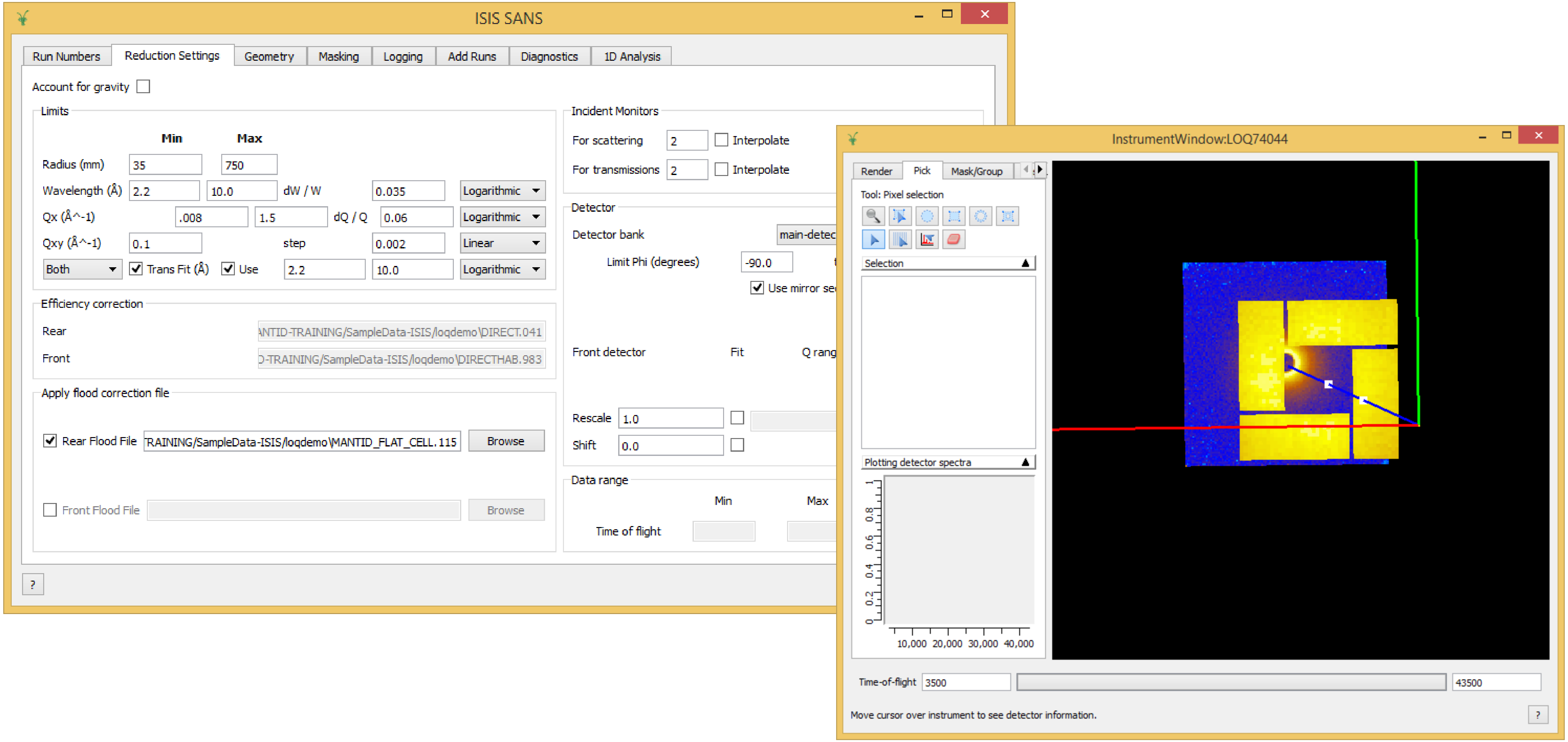
Usability:

- 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, Grasp & Mantid interfaces → what should be changed?)

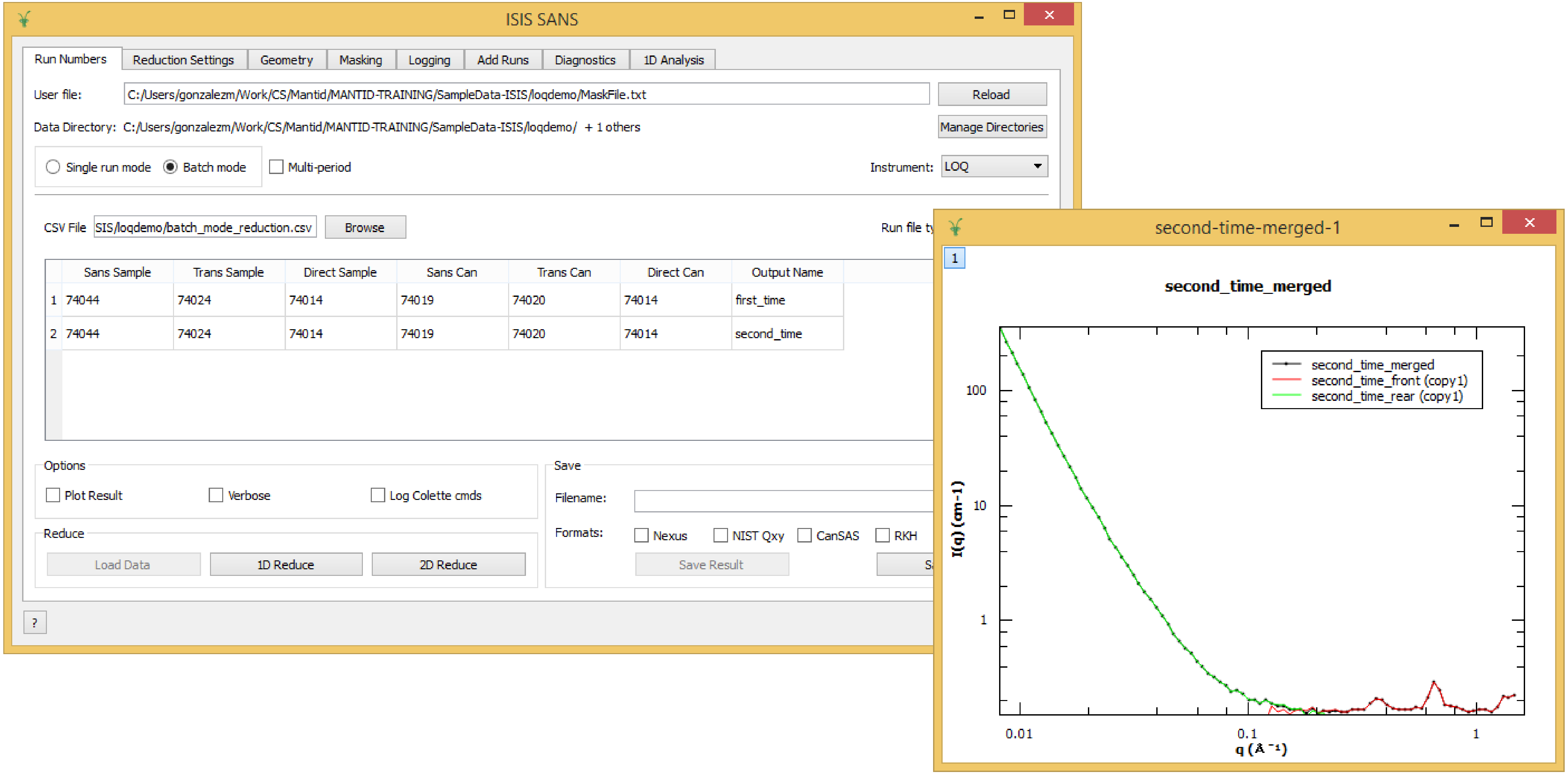
"Quality" control:

- Set of reference measurements that can be used to cross-check?
- Benchmark with existing software (LAMP/Grasp)
- Generate an artificial 'perfectly known' data set?

BASTILLE-MANTID SANS DISCUSSION – EXAMPLE FROM MANTID



BASTILLE-MANTID SANS DISCUSSION – EXAMPLE FROM MANTID



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

- Standard/classic SANS mode (D11/D22/D33) - isotropic
- Standard/classic SANS mode (D11/D22/D33) – 2D
- TOF SANS mode (D33) - isotropic
- TOF SANS mode (D33) – 2D
- Kinetic scans
- Event mode data – D22 (more general than Tisane)
- Polarized neutrons (D33)
- ‘Imaging’
- Additional macros/tools in LAMP/IDL/Grasp ?
- Case D16 (as for SANS 1D and 2D, but also detector scans and rocking curves BUT not always direct beam on the detector)

Note: Logically isotropic and 2D methods should be ‘inverted’, isotropic SANS being a special case of 2D SANS

Method 1. General SANS mode (D11/22/33): data – 2D: (Q_X-Q_Y), 1D output – I(Q)

1. *Read data (NeXus):
   1. sample (S),
   2. direct beam (D), optional additional direct beam (OD) for broader collimation setting,
   3. Instrument (blocked beam) background (IB),
   4. empty cell (EC),
   5. ‘water’ (calibration) data; sample (WS), direct beam (WD), empty cell (WEC) - optional,
   6. transmission data for direct beam (TD), empty cell (TEC), sample (TS), water (TW) OR known values
2. Data calibrated from calibration file if exists/used - optional
3. *Correct detector dead time (given formula for instrument) for S, D and transmission files
4. Additional input: sample thickness (also water thickness)
5. Create detector mask and beamstop mask – default masks per instrument OR define manually
6. *Determine SANS centre and beam width (for Q resolution) from D
7. *Calculate transmission values for sample and empty cell from transmission data (TD, TEC, TS) - .
8. *Subtract cell (S-EC) using transmission value as a function of scattering angle and monitor values.
9. *Subtract instrument background (S-IB) using transmission value as a function of scattering angle and monitor values.
10. *Correct sample (S-EC-IB) for solid angle, sample thickness, parallax (instrument dependent)
11. If using water (rather than a calibration file), repeat steps 6, 7, 8, 9, 10
12. *Absolute scaling: water scaling (using water cross-section) OR scaling using estimated incident flux
13. *Integrate data: radial (using beam centre, determine Q resolution)
14. *Merge data for different Q ranges (& Q resolutions) from detector positions or TOF mode

Method 1 (cont). General SANS mode (D11/22/33): data – 2D: (Q_X-Q_Y), 1D output – I(Q)

See e.g. 'live_sans_reduction.prox' in LAMP.

Be careful with steps in method if not all data is available or used.

'Gravity correction' needed for D33 since detectors (front & back) not at same distance

D33 – may need to select detector panels independently

Method 2. General SANS mode (D11/22/33): data – 2D: (Q_X-Q_Y), 2D output – I(Q_X,Q_Y)

As for method 1 until step 13 – radial integration replaced by e.g. integration by sectors

OR output 2D data and fit e.g. in SASview.

Anything else that is different?

Rocking curves on initial data set to align sample?

Need to merge 2D data on D16 (different detector angles)

Method 3. TOF mode (D33): data – 3D: (Q_X-Q_Y, TOF), 1D output – I(Q)

As for method 1 looping through TOF channels which give different Q ranges with different Q resolutions.

Flexibility required for rebinning data and selecting data ranges (if for example, longest wavelength data does not have useful statistics)

Possibly merging 2D data (OK for 1D data)

Gravity correction needed for each wavelength

Method 4. TOF mode (D33): data – 3D: (Q_X-Q_Y, TOF), 2D output – I(Q_X,Q_Y)

As for method 2 looping through TOF channels which give different Q ranges with different Q resolutions.

Method 5. Kinetic mode: data – 3D: (Q_X-Q_Y, time) or 4D (Q_X-Q_Y, TOF, time), 2D output – I(Q, time), 3D output I(Q_X, Q_Y, time)

As for methods 1 & 2 looping through time channels

Flexible rebinning of time step data required

Kinetic measurements account for less than 10% of measurements

Method 6. Event mode (D22 - Tisane): data – events rather than histograms in Q, TOF, time, etc

Current thinking 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.

Also needed on D11 and D33

Method 7. Polarised neutrons: data – as any other data set with, in addition, different polarisation states

Can data from different polarisation states be treated independently and then the reduced combined?

Standard reduction needs to take into account partial polarisation of beam and time dependence of 3He polariser as extra steps in standard treatment - method 1 (see module in Grasp - Dirk)

Several experiments per cycle use polarised neutrons, this fraction is increasing…

Method 8. ‘Imaging’

Scanning a small aperture/beam across the sample

2 experiments so far

ALGORITHMS for SANS (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)

1.5 *Determine SANS centre and beam width (for Q resolution) from Direct beam

Data: 2D(Q_X,Q_Y) – fit or numerically determine (first moment) direct beam, see e.g. sans_center in sans_setting.pro (Lamp)

1.6 * Calculate transmission values for sample and empty cell from transmission data (TD, TEC, TS)

Data: 2D(Q_X,Q_Y) – see e.g. sans_transm in sans_setting.pro (Lamp)

1.7 *Correct detector dead time (given formula for instrument)

Data: 2D(Q_X,Q_Y) – see e.g. sans_tau in sans_setting.pro (Lamp)

1.8, 1.9 & 1.10 * Subtract cell (EC) using transmission value as a function of scattering angle and monitor values & Correct for solid angle, sample thickness, parallax (instrument dependent)

Data: 2D(Q_X,Q_Y) – see e.g. sans_cor in sans_setting.pro (Lamp) ?

1.12 * Absolute scaling

Data: 2D(Q_X,Q_Y) – output data on absolute (rather than arbitrary scale) see e.g. sans_cor in sans_setting.pro (Lamp) ?

1.13 *Integrate data

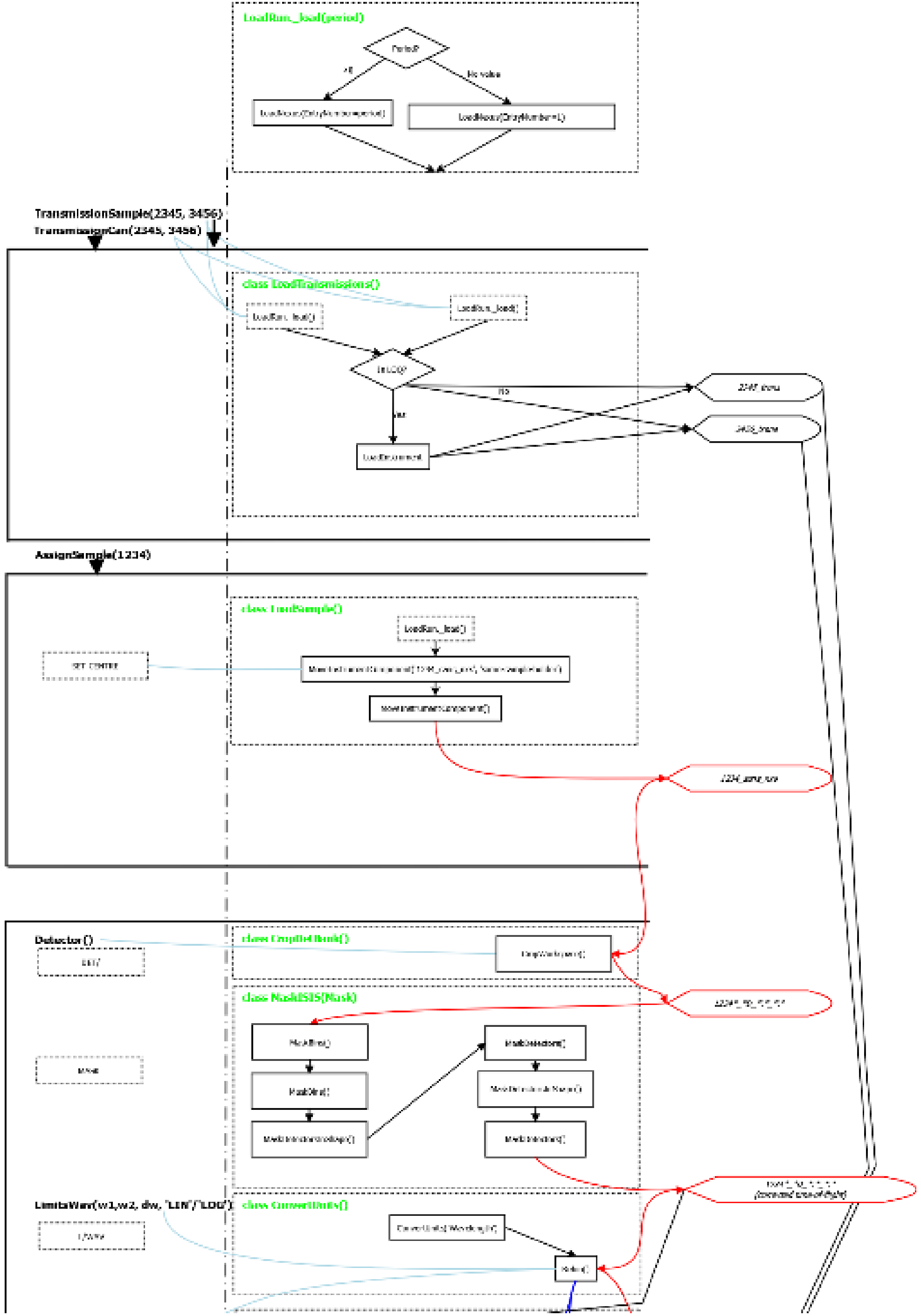
Data: 2D(Q_X,Q_Y) – radial integration => I(Q), see e.g. sans_radial in sans_setting.pro (Lamp)

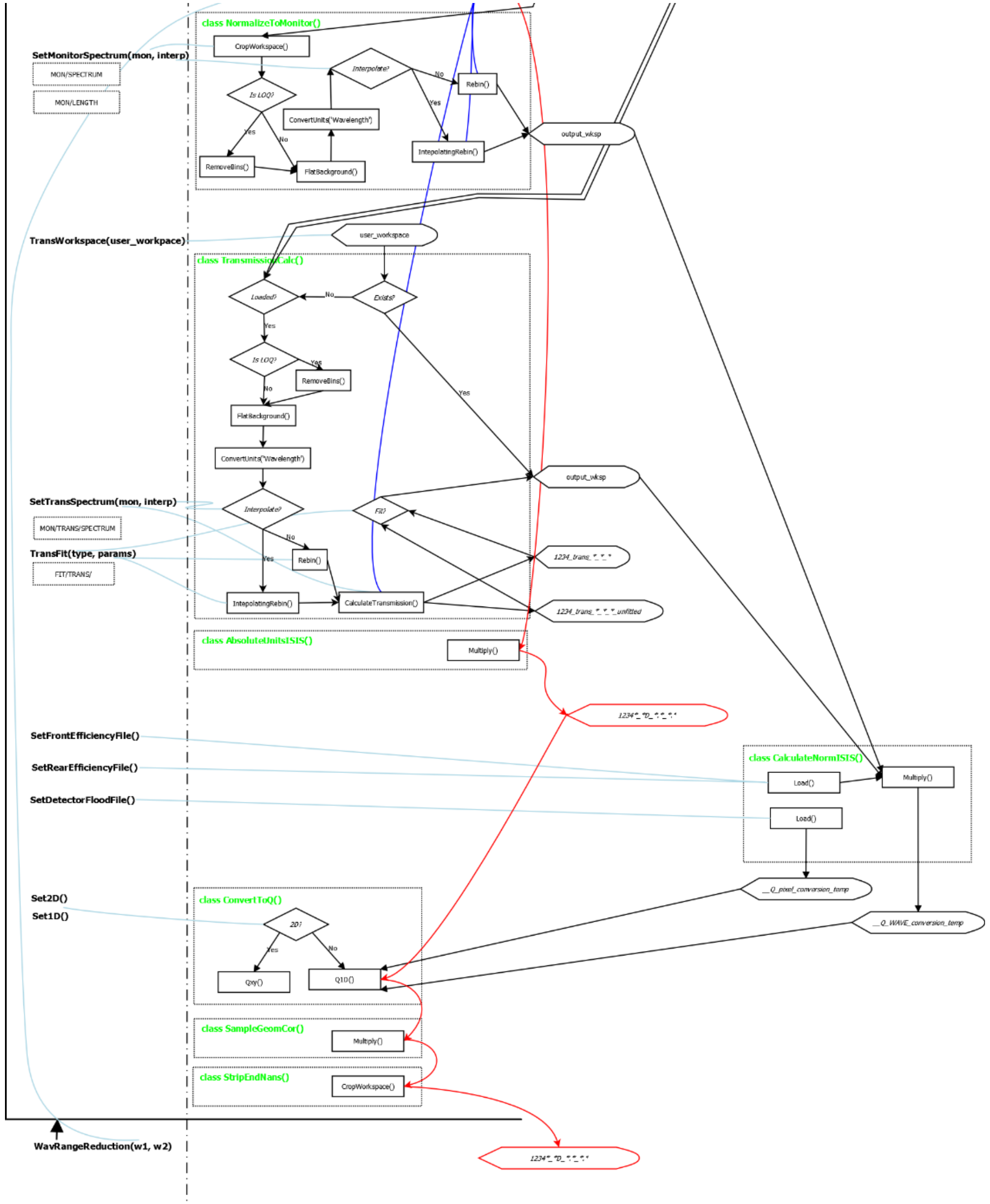
1.14 *Merge data

Data: 1D(Q) – merge data covering different Q ranges, see e.g. sans_merge in sans_setting.pro (Lamp)

Document/details (possibly with flowcharts) to be completed by Dirk (and LSS and CS if necessary) in one month (~ April 25 2015)

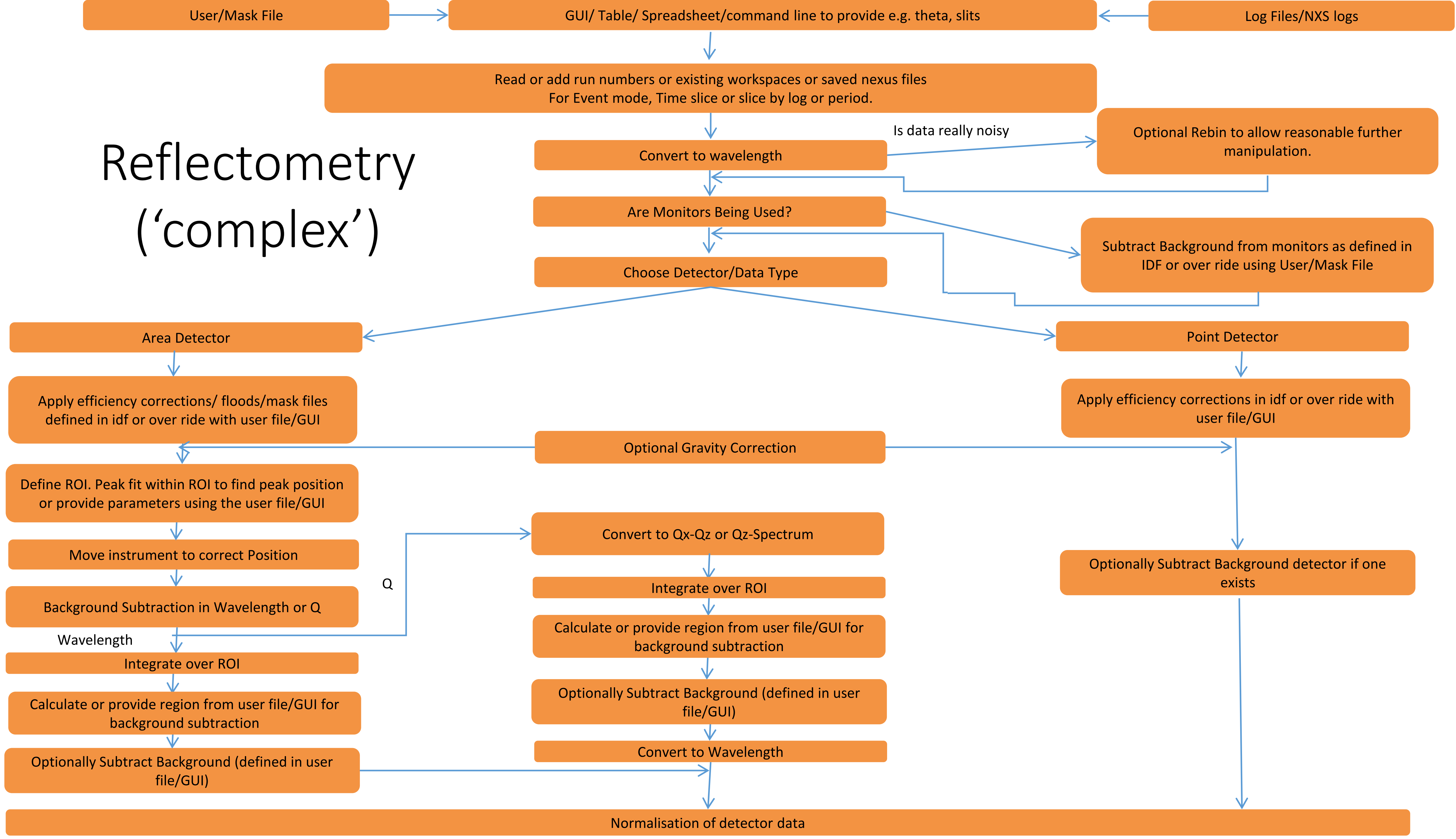
The following flowchart is for SANS@LOQ/ISIS – it shows an appropriate level of detail and how different methods can be combined in a single application or GUI



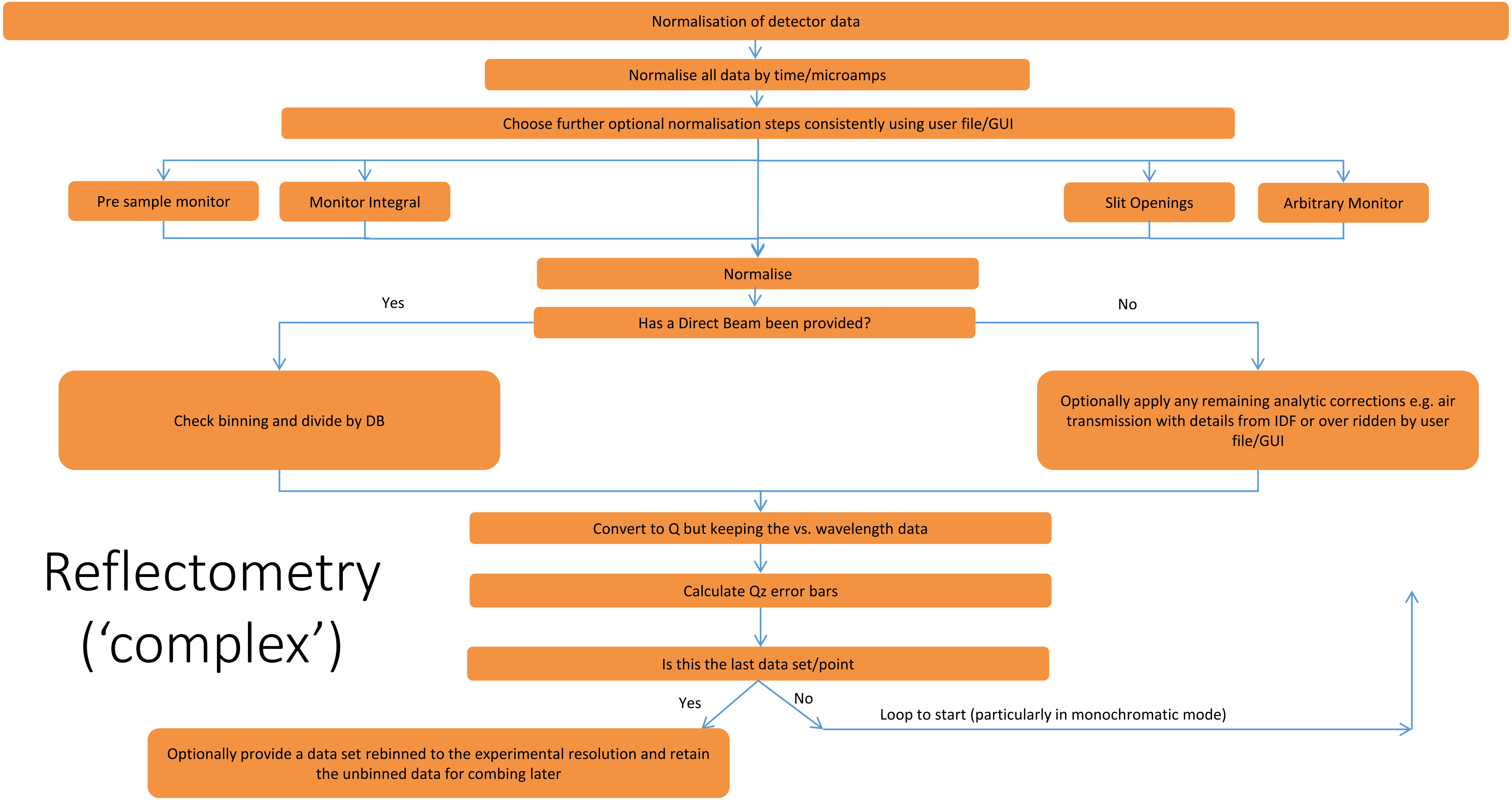


http://www.mantidproject.org/images/8/8f/ISIS_SANS_reduction.png

The following 'reflectometry' flowchart is another example of how different methods can be combined in a single application or GUI


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