BASTILLE-MANTID-COSMOS DISCUSSION

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

2. Scope:

Write set of workflows for each reduction-type (TOF, 2T, kinetic, polarised,…):

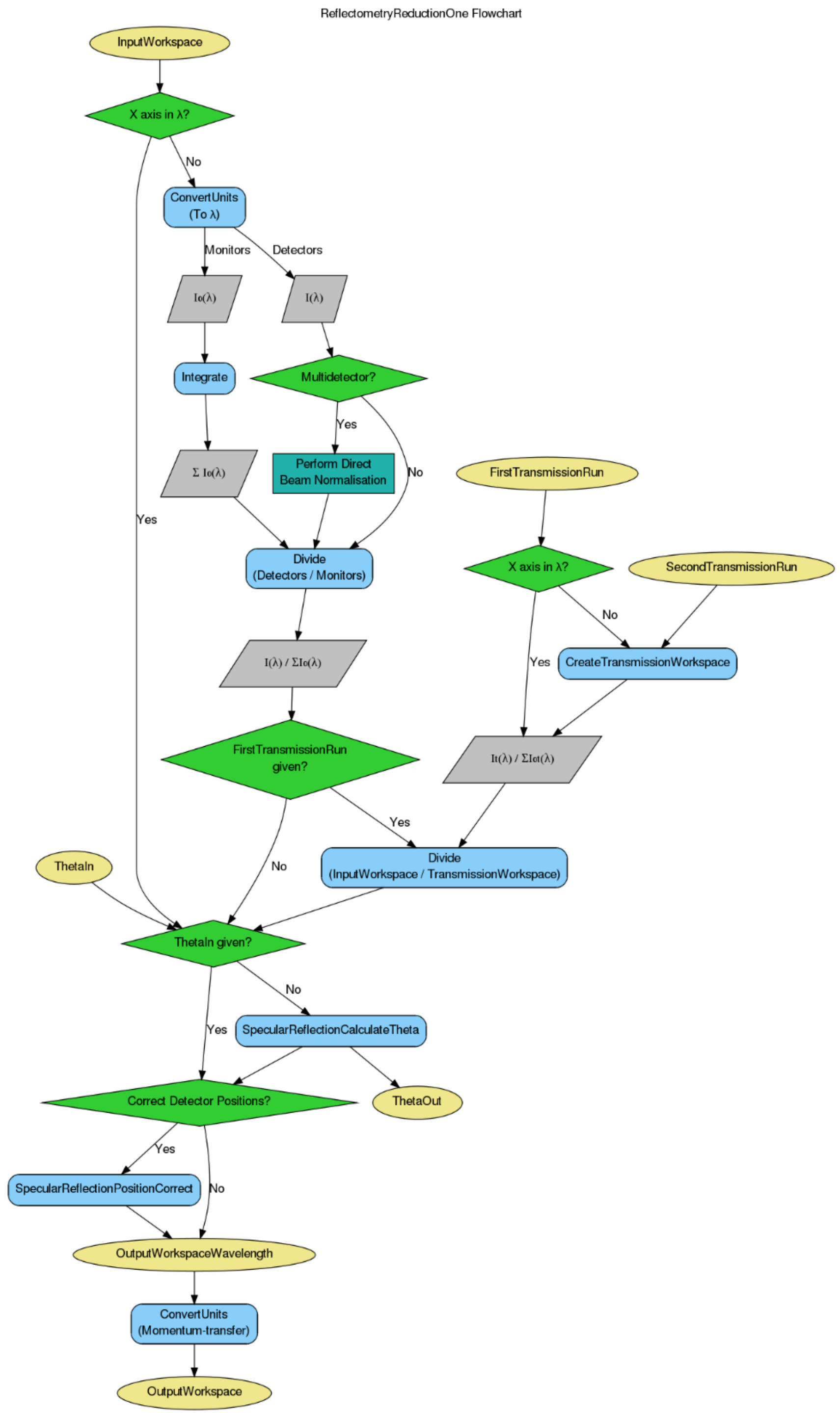
- *Existing and future workflows*
- *Short description of algorithm/calculation for each step*
- *Does everyone agree on steps/order for a given reduction type*

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: Cosmos & Mantid interfaces → what should be changed?)

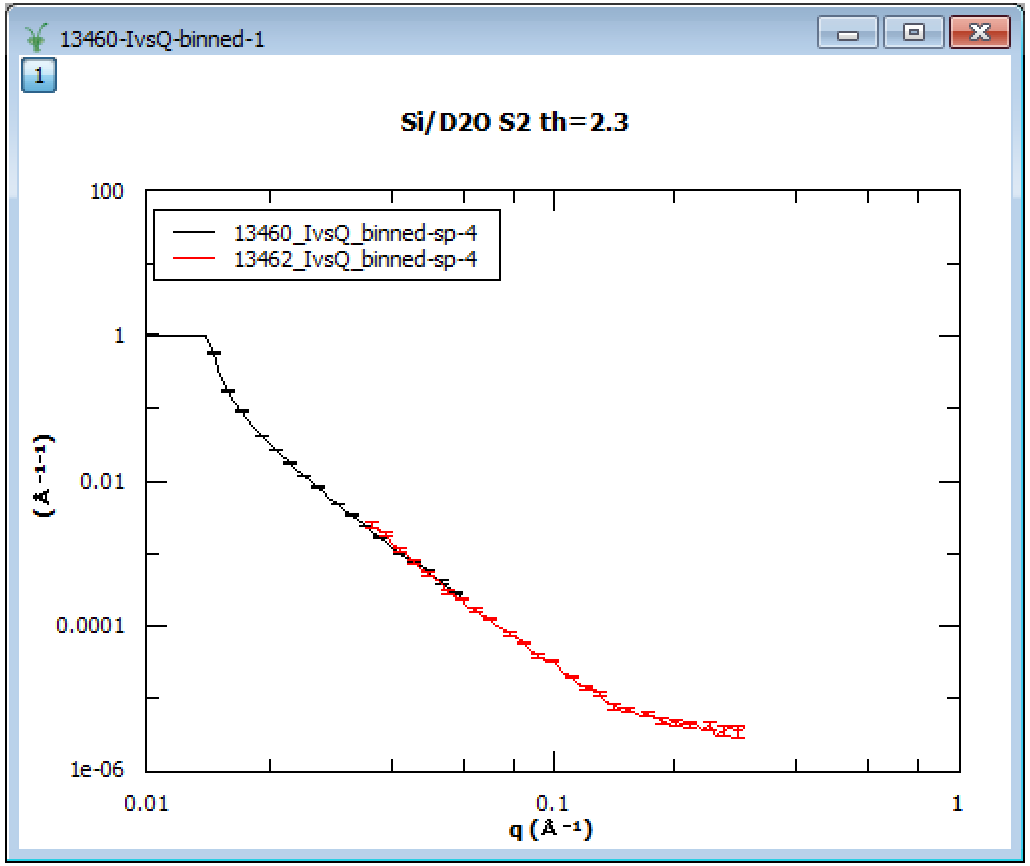
“Quality” control:

- Set of reference measurements that can be used to cross-check?
- Comparison to existing software (but e.g. note that different versions of Cosmos may give different results, as resolution calculations and ways of grouping the data have evolved)
- Generate an artificial ‘perfectly known’ data set?



	Run(s)	Angle 1	trans 1	qmin_1	qmax_1	Run(s)	Angle 2	trans 2	qmin_2	qmax_2	Run(s)	Angle 3	trans 3	qmin_3	q
1	13460	0.7	13463...	0.01	0.06	13462	2.3	13463...	0.035	0.3					
2	13469	0.7	13463...	0.01	0.06	13470	2.3	13463...	0.035	0.3					
3															

	1	Run(s)	Angle 2	trans 2	qmin_2	qmax_2	Run(s)	Angle 3	trans 3	qmin_3	qmax_3	dq/q	Scale	Stitch?	Plot?
1		13462	2.3	13463...	0.035	0.3						0.04			Plot
2		13470	2.3	13463...	0.035	0.3						0.04			Plot
3															Plot



Determine current and future needs/types of analysis:

- Standard TOF mode (D17/FIGARO) = Cosmos
- Kinetic scans in TOF mode (D17/FIGARO) = Cosmos/Galaxy
- 2θ mode (D17): %use? How are those data reduced/handled today? SuperADAM (CRG)?
- 3D numors (θ_x,θ_y,TOF): Read & visualization in Lamp. Any treatment?
- Polarized neutrons (D17): To come in Cosmos. Treatment today?
- Macros/tools in LAMP/IDL (Bob, Andrew): What is needed? Context of use?
- Event mode data?
- …?

Method 1. Standard TOF mode (D17/FIGARO) : data – 2D: (2theta – TOF)

1. *Read data (NeXus): sample – reflected beam (R), direct beam (D), instrument background (IB), 'water' (calibration) data (W), D_2O (normalisation data)
2. Correct R, D, IB data for detector efficiency: divide/multiply by W or calibration data from file
3. Normalise to monitor or counting time (and different slits openings if needed)
4. (check input parameters – from data files and user input)
5. Subtract instrument background: R-IB and D-IB
6. *Find reflected peak (Region of Interest – ROI_peak) in R and D
7. *Determine background ROI_back in R and D
8. Subtract (average) background: (R-IB)_fore – (R-IB)_back and (D-IB)_fore – (D-IB)_back
9. *Determine θ and λ
10. *Correction for gravity (Figaro) → new θ and λ
11. Integrate ROI (order – swap?): Total_(R-IB)_back and Total_(D-IB)_back [1D vectors]
12. Divide reflected beam by direct beam → Reflectivity
13. *Convert Lambda → Q and determine dQ
14. *Q rebin based on Q, dQ
15. Multiply by normalisation/scaling factors (related to collimation, attenuators, fraction of reflected beam,…)
16. Join measurements with different θ
17. Plot reduced data
18. Write reduced data in required formats

*specific algorithms for reflectometry (other operations/algorithms are part of framework)

NB. Kinetic scans involve the above treatment repeated for all time-dependent data sets

Method 2. theta-2theta scans, no TOF (e.g. SuperAdam: data – 2D: (Q_X-Q_Y))

1. *Read data (NeXus): sample – reflected beam ($R(\theta)$), direct beam (D), and efficiency file (W)
2. Correct R and D for detector efficiency: divide/multiply by calibration file
3. Normalise to monitor or counting time
4. Compute Q values
5. Integrate over ROI in 2D detector → Total counts for each Q (in R and D)
6. R(Q)/D

Method 3. Polarisation analysis

1. - 12. As in Method 1, but repeated for 2, 3 or 4 measurements with different polarizations (e.g. I^{00}, I^{01}, I^{10}, I^{11})

13. *Correct instrument polarization effects → Σ^{++}, Σ^{+-}, Σ^{-+}, Σ^{--}

14. Convert Lambda → Q and determine dQ

15. Q rebin based on Q, dQ

16. Multiply by normalisation/scaling factors (related to collimation, attenuators, fraction of reflected beam,…)

17. Join measurements with different θ

18. Plot reduced data

19. Write reduced data in required formats

ALGORITHMS – specific for reflectometry (complete with references, equations, existing algorithms, etc)

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

1.6 *Find reflected peak (Region of Interest – ROI_peak)

Data: 2D(θ, TOF) – integrate over TOF & fit I(θ) to find θ_{min} and θ_{max} OR set θ and TOF limits manually

1.7 *Determine background ROI_back

2 ROI defined manually as shift from reflected peak, background taken as simple average from 2 ROIs or linear fit from 2 ROIs

1.9 *Determine θ and λ (if using peak position in detector – D17 only)

Instead of taking θ from table or data file, find peak position in detector and calculate θ from detector position, correcting for sample-detector distance

1.10 *Correction for gravity (Figaro)

Calculate effective θ at sample surface and λ for longer beam path

1.13 *Convert Lambda → Q and determine dQ

Basic formula is Q=4pi.sin(θ)/ λ , dQ depends on numerous parameters

1.14 *Q rebin based on Q, dQ

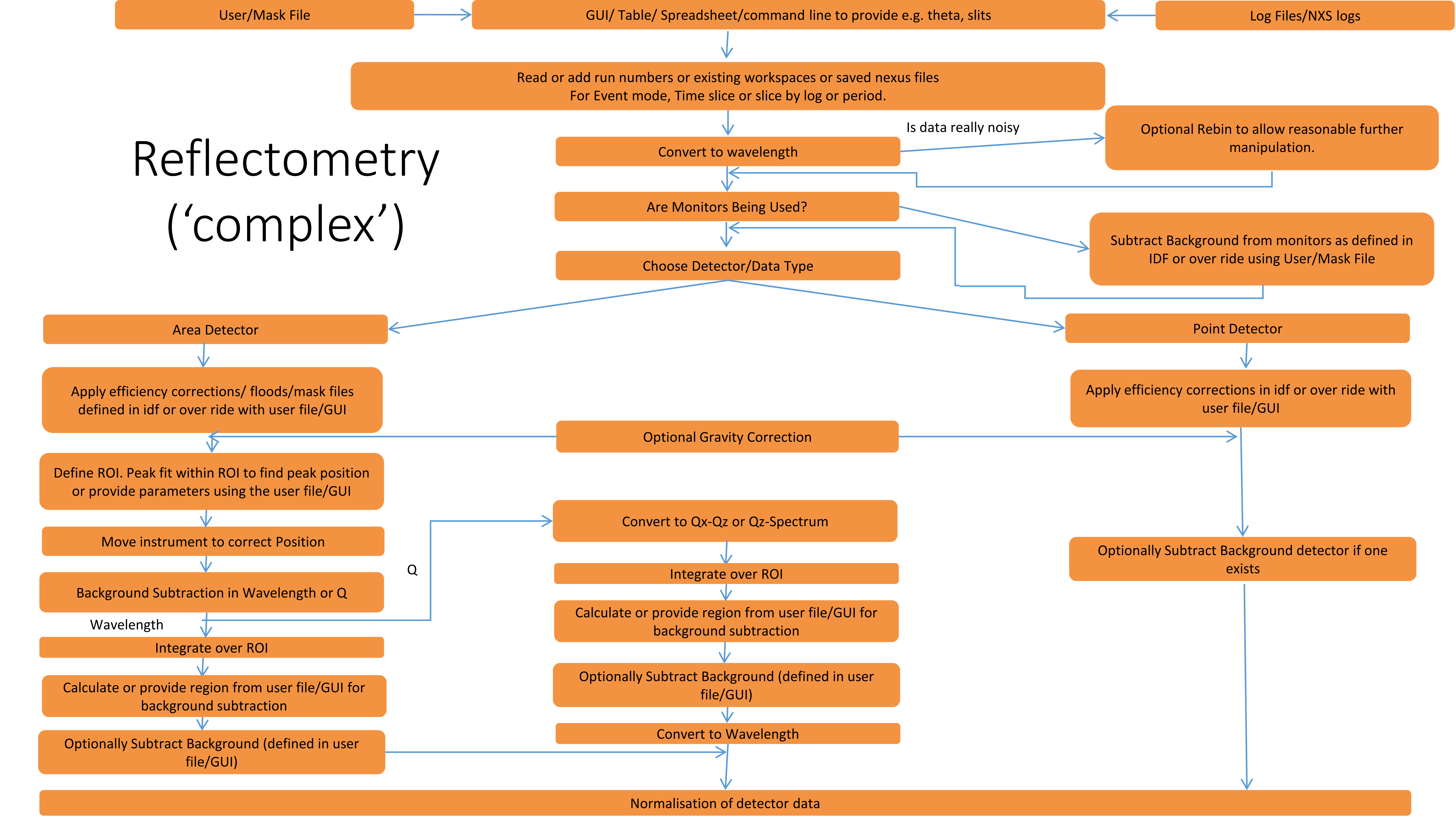
Improve statistics by reducing number of points, taking into account dQ

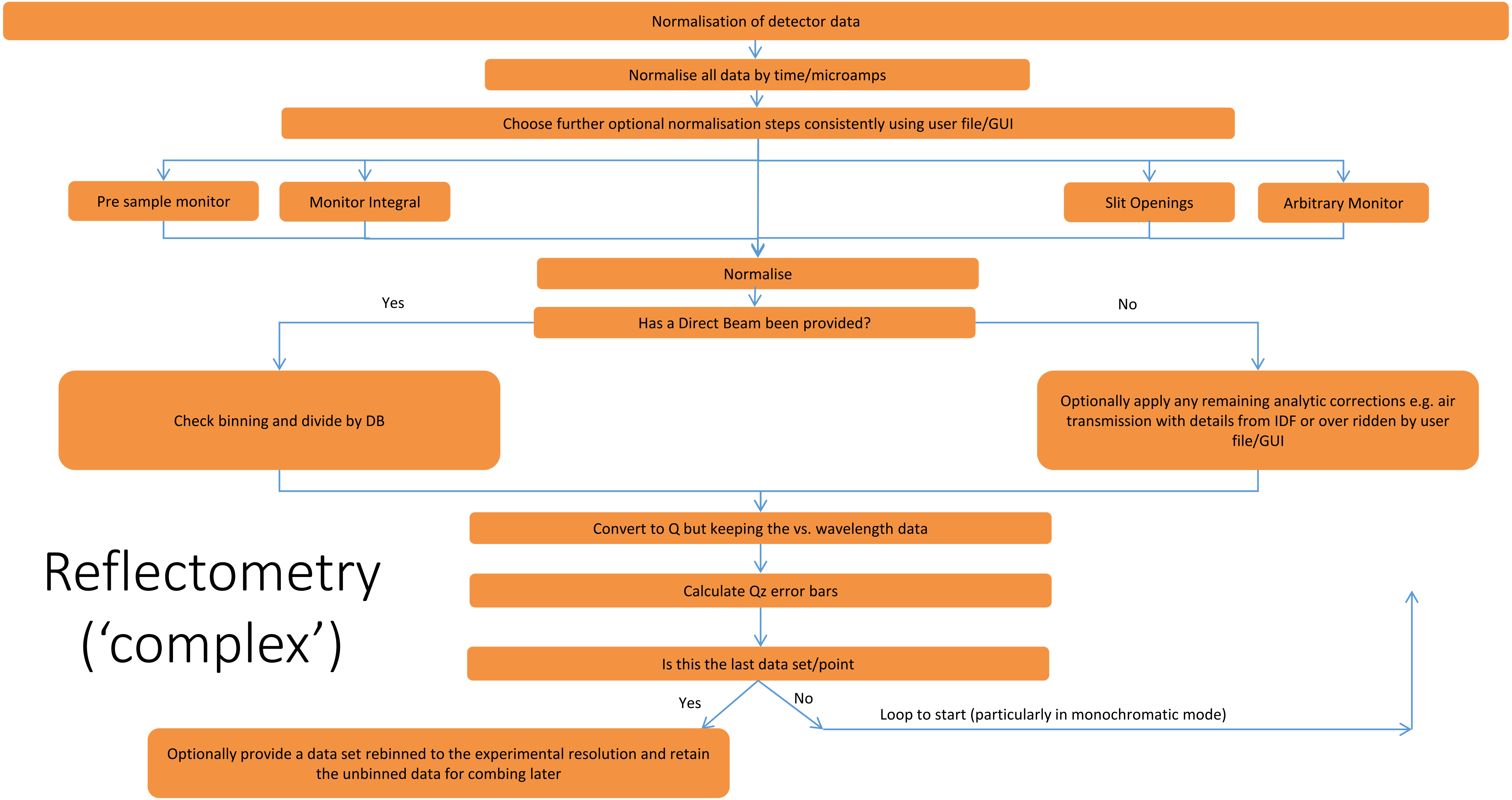
2.1 *Read data (NeXus): data – 2D: (Q_X-Q_Y)

3.13 *Correct instrument polarization effects → Σ^{++}, Σ^{+-}, Σ^{-+}, Σ^{--}

Wildes, Rev. Sci. Instrum., 70 (1999) 4241

Document/details (possibly with flowcharts) to be completed by Thomas (and LSS and CS if necessary) in one month (~ April 17 2015)


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
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
Integrate over ROI
Calculate or provide region from user file/GUI for background subtraction
Optionally Subtract Background (defined in user file/GUI)
Normalisation of detector data



Reflectometry ('complex')

→ CLEAR, COMPLETE REQUIREMENT DOCUMENT

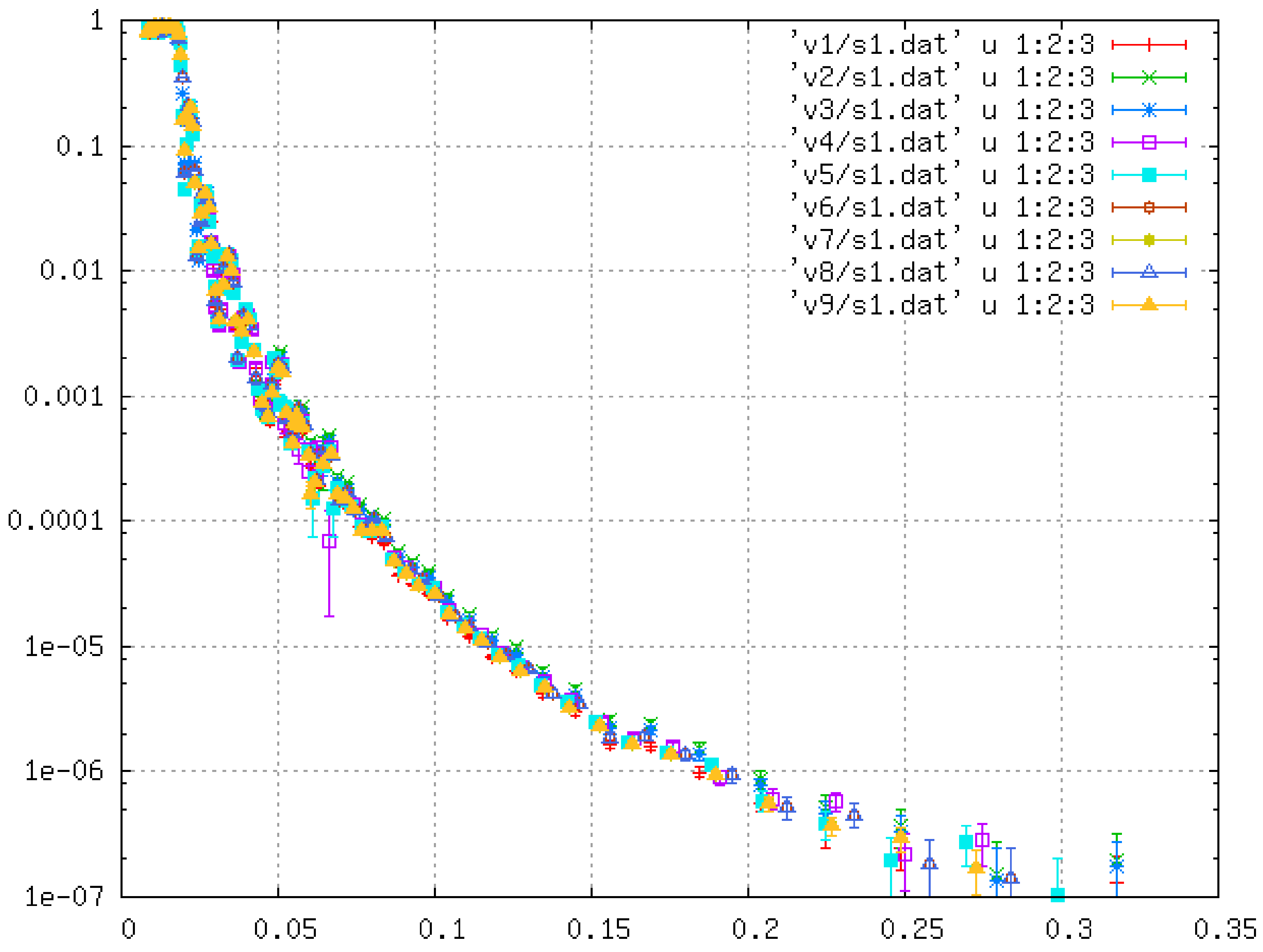
3. Cosmos 2015:

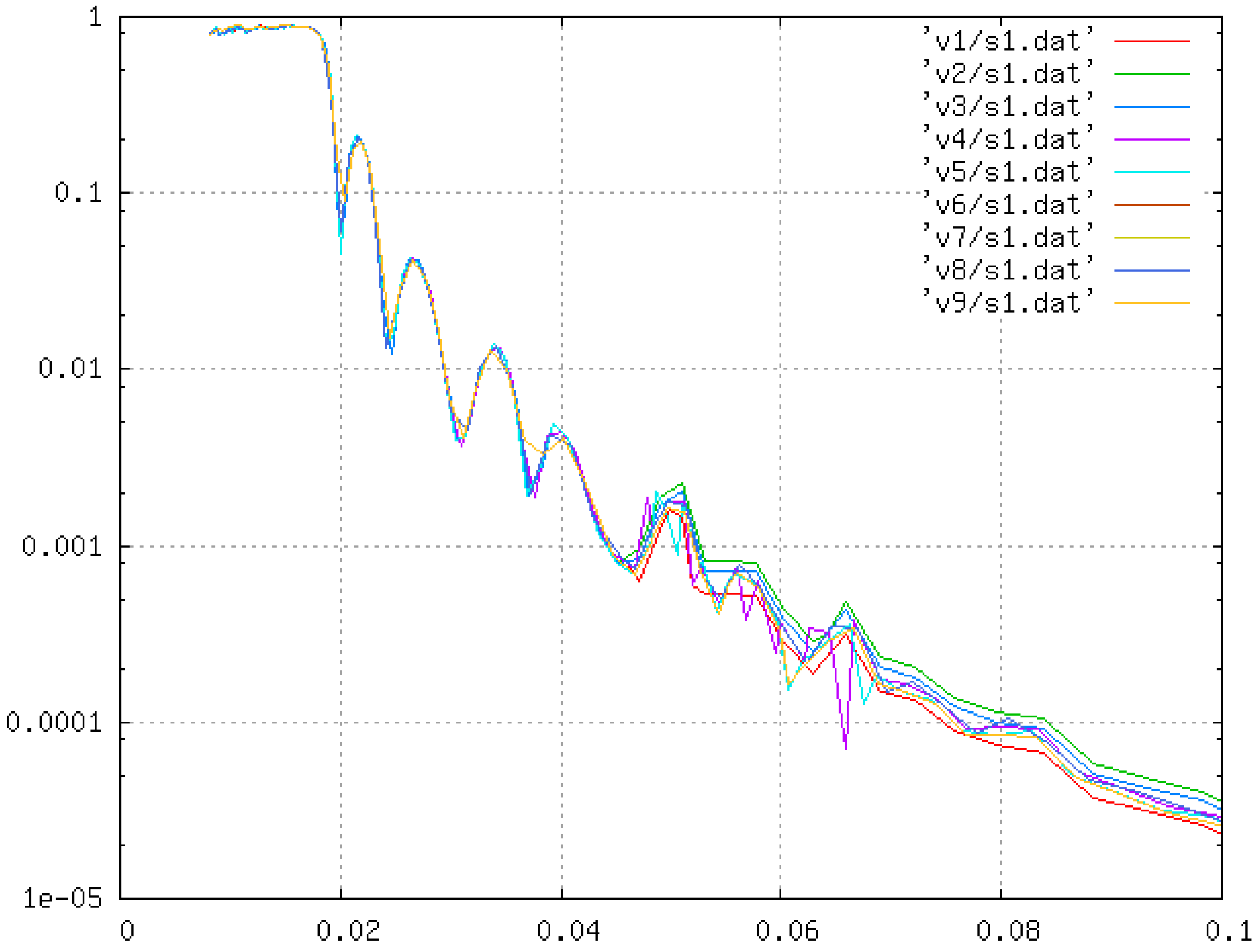
- Inform everybody on ongoing developments and agree on choices.
- Cleaning and increase performance (e.g. avoid re-reading repeatedly same DB files):
  - Any interest in handling rows without a RB?
  - Monitor_run: A DB numor is given (as M 123456), but the incident flux is determined from monitor and not from detector. To maintain?
  - What to do if no DB given? (Now Figaro will use the monitor of the RB to estimate flux(λ), D17 will stop; in pre-Figaro Cosmos I think that it would go ahead with background subtraction and foreground integration and give I(λ))
  - "Useless" (same info repeated) columns?
- Read Nexus files:
  - Use read_hdf.pro (from Lamp)
- Coherent analysis:
  - Calculation tab: Foreground given now as a couple of integers indicating the number of pixels to take to the left (below) and to the right (above) of the pixel corresponding to the peak position. Old format (a single integer) will work, but the table will be saved with two integers (i.e. 13 will appear as 6,6).
  - New resolution calculation (Bob, Philipp): In 'incoherent' treatment, you could have the message *Row 1: The sample is bent! Use constant q foreground COSMOS!* appearing for each treated row and angle.
  - The Q resolution has now a dependency on the counting in the detector (unsatisfactory?) → need to solve this, as it breaks the treatment of kinetic numors.

- Polarization:
    - Change in Cosmos logics (cosmos_anal_run treats a single angle from a row)
    - Are all 'rows' and 'angles' similar (same polarization measurements or can they be mixed)?
        - Drop down menu in Data tab to select polarization mode (non-polarized, full polarized, spin-flip etc)
    - Changes in the user interface:
        - Extra columns to account for different polarization measurements
        - Different polarizations in different rows (1 row $\neq$ 1 sample)
        - Different polarizations in same cell, but column header becoming a drop down menu allowing to cycle between the polarizations (confusing?, more complex?)

- Update documentation:
    - Help for users/tutorial (update webpages?)
    - Better description of treatment performed: workflow, details on how operations are performed (peak search, background subtraction), equations (resolution calculation)

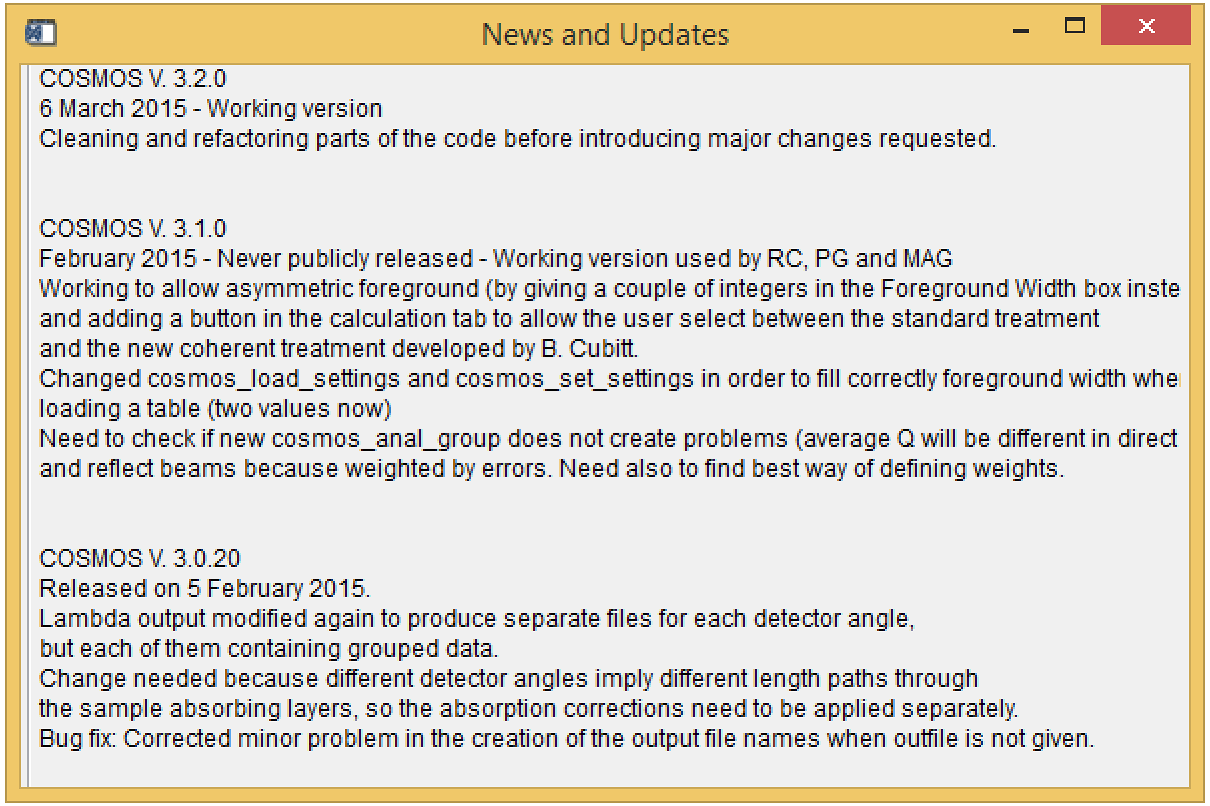
- Validation:
    - To check gravity corrections
    - Set of reference measurements to validate each version


1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
'v1/s1.dat' u 1:2:3
'v2/s1.dat' u 1:2:3
'v3/s1.dat' u 1:2:3
'v4/s1.dat' u 1:2:3
'v5/s1.dat' u 1:2:3
'v6/s1.dat' u 1:2:3
'v7/s1.dat' u 1:2:3
'v8/s1.dat' u 1:2:3
'v9/s1.dat' u 1:2:3



1
0.1
0.01
0.001
0.0001
1e-05
0
0.02
0.04
0.06
0.08
0.1
'v1/s1.dat'
'v2/s1.dat'
'v3/s1.dat'
'v4/s1.dat'
'v5/s1.dat'
'v6/s1.dat'
'v7/s1.dat'
'v8/s1.dat'
'v9/s1.dat'

Changes in Cosmos:



News and Updates

COSMOS V. 3.2.0
6 March 2015 - Working version
Cleaning and refactoring parts of the code before introducing major changes requested.

COSMOS V. 3.1.0
February 2015 - Never publicly released - Working version used by RC, PG and MAG
Working to allow asymmetric foreground (by giving a couple of integers in the Foreground Width box inste
and adding a button in the calculation tab to allow the user select between the standard treatment
and the new coherent treatment developed by B. Cubitt.
Changed cosmos_load_settings and cosmos_set_settings in order to fill correctly foreground width whe
loading a table (two values now)
Need to check if new cosmos_anal_group does not create problems (average Q will be different in direct
and reflect beams because weighted by errors. Need also to find best way of defining weights.

COSMOS V. 3.0.20
Released on 5 February 2015.
Lambda output modified again to produce separate files for each detector angle,
but each of them containing grouped data.
Change needed because different detector angles imply different length paths through
the sample absorbing layers, so the absorption corrections need to be applied separately.
Bug fix: Corrected minor problem in the creation of the output file names when outfile is not given.

Bugs/Requests:

gonzalezm@ill.fr

https://forge.epn-campus.eu/projects/lamp/issues (Register in https://forge.epn-campus.eu/account/register and write to me to include you as a project reporter, so that you can raise new issues)