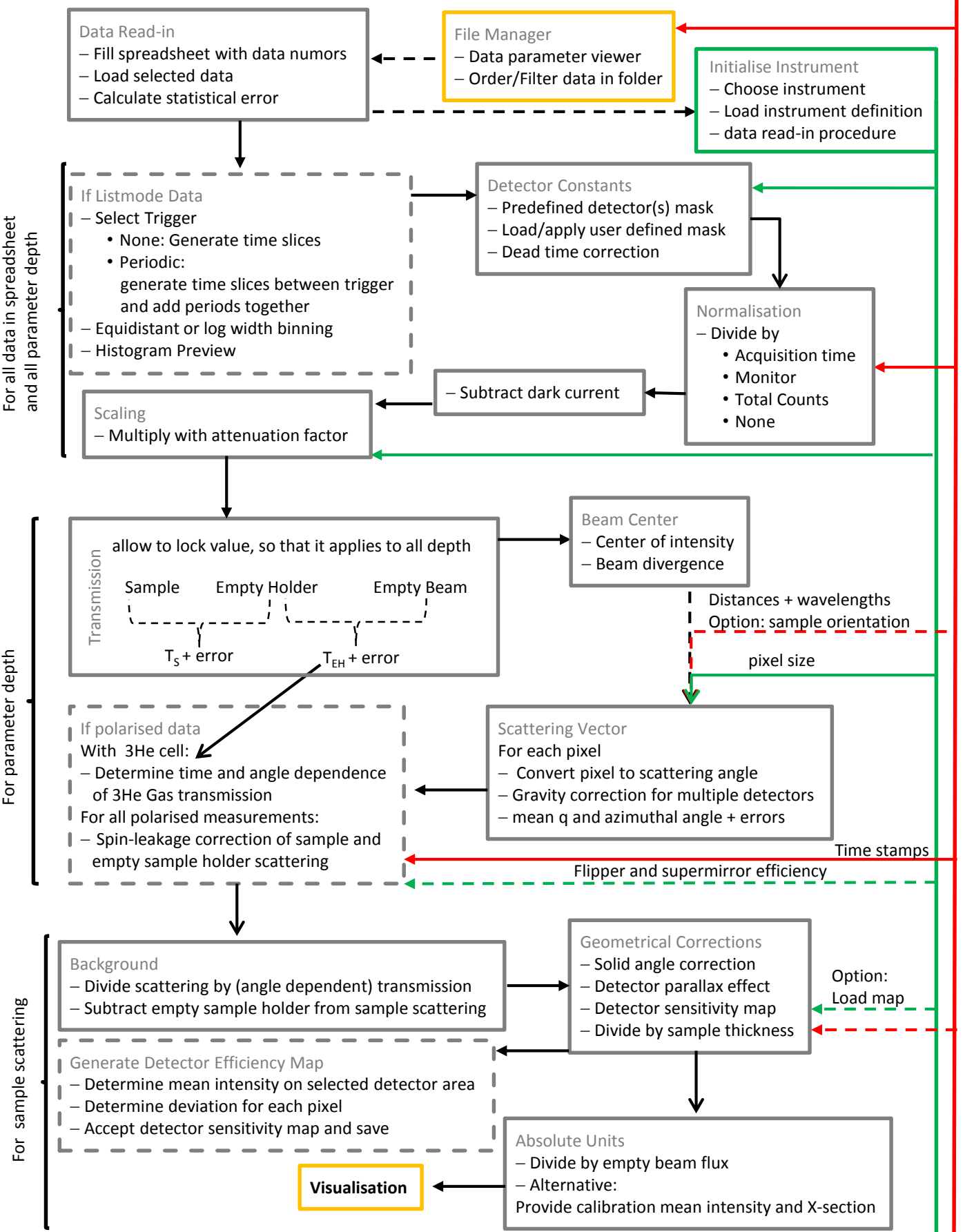# Data reduction workflow

Note: Dashed boxes are optional, a dashed path can be overridden by user input

Dataparams

Data Read-in
– Fill spreadsheet with data numors
– Load selected data
– Calculate statistical error

File Manager
– Data parameter viewer
– Order/Filter data in folder

Initialise Instrument
– Choose instrument
– Load instrument definition
– data read-in procedure

For all data in spreadsheet and all parameter depth

If Listmode Data
– Select Trigger
  • None: Generate time slices
  • Periodic:
    generate time slices between trigger
    and add periods together
– Equidistant or log width binning
– Histogram Preview

Detector Constants
– Predefined detector(s) mask
– Load/apply user defined mask
– Dead time correction

Normalisation
– Divide by
  • Acquisition time
  • Monitor
  • Total Counts
  • None

– Subtract dark current

Scaling
– Multiply with attenuation factor

For parameter depth

Transmission

allow to lock value, so that it applies to all depth

Sample   Empty Holder   Empty Beam

T_S + error T_{EH} + error

Beam Center
– Center of intensity
– Beam divergence

Distances + wavelengths
Option: sample orientation

pixel size

If polarised data
With 3He cell:
– Determine time and angle dependence
  of 3He Gas transmission
For all polarised measurements:
– Spin-leakage correction of sample and
  empty sample holder scattering

Scattering Vector
For each pixel
– Convert pixel to scattering angle
– Gravity correction for multiple detectors
– mean q and azimuthal angle + errors

Time stamps

Flipper and supermirror efficiency

For sample scattering

Background
– Divide scattering by (angle dependent) transmission
– Subtract empty sample holder from sample scattering

Geometrical Corrections
– Solid angle correction
– Detector parallax effect
– Detector sensitivity map
– Divide by sample thickness

Option:
Load map

Generate Detector Efficiency Map
– Determine mean intensity on selected detector area
– Determine deviation for each pixel
– Accept detector sensitivity map and save

Visualisation

Absolute Units
– Divide by empty beam flux
– Alternative:
Provide calibration mean intensity and X-section

Data Worksheet

The Data Reader GUI should have the appearance of a spreadsheet (e.g. LAMP), so that the user has at one glance an overview of the required information (sample and background scattering/transmission, dark current) and already given run numbers. The spreadsheet should provide space for complementary instrument configuration (e.g. detector positions) and should allow to add new rows to append several samples.

In general, each run can contain parameter frames (axis/wavelength/time slices). Features like adding series of runs (summing intensities +total acquisition time/monitor of equivalent frames) as well as concenating runs in parameter frame depth have to be supported.

Spin-leakage correction

As a prerequisite for spin leakage correction, data (optionally user) has to provide a flag for the experiment [polarised beam only (SANSPOL) or polarisation analysis (POLARIS)] and the order of spin states in parameter depth. Algorithms for spin leakage correction for SANSPOL (i.e. 2 spin states) and POLARIS (4 spin states) can be found in /grasp/polarisation analysis/sanspol_correct.m and pa_polarisation_correct.m respectively. Note that using a 3He cell the correction factors are time-dependent. These factors are given by the time evolution of the transmission without sample in beam.

Visualisation

Basic functionalities for graphical output should comprise:
Data point selector/cursor
Zoom function
Select displayed detector area as ROI or mask

For processed 2D detector data:
Scroll through depth
Movie function in depth (e.g. along time dimension or instrument parameter)
Optional: store results as annotation in Nomad logfile (logs.ill.fr)

Visualisation
Show processed 2D detector data
Option: allow basic operations (add, subtract, divide) with other 2D data set

Region of Interest (ROI)
− Define ROI (lines/ring segments/rectangles/frames) relative to beam center
− Selected/deselect whole detectors
Option: allow basic operations for ROI (union/intersection ..)

Error estimation for ROI
Implement feedback to NOMAD, which than takes decision, e.g.
- if error > threshold measure another set
- deviation between two sets < threshold go to next parameter value (temperature/field..)...

Binning
− Boxes: Integrate intensity in ROI
− Bin azimuthal angle: radial/sector average
− Q binning: Equidistant or log width

Mask
− User defined mask

evaluate accordingly selected depths and configuration data

Grouping + Merging
− Group data as data set
− Interpolate for multiple points on same Q-interval
Allow for a single depth/configuration:
− Scale data by multiplication factor
− Hide data points at beginning and end of Q-interval

Reduced Data
2D output:
− I vs q or azimuthal angle
− Sum in ROI vs instrument parameter or time
3D output (for non-grouped data):
− I vs $|q|$ or azimuthal angle and instrument parameter or time
− Sum vs instrument parameters (raster image)
− I vs (q_y, q_z) or ($|q|$, azimuthal angle)