Software requirements for reflectometry

# Main instrument controll (reference pyDAS@SNS, gumtree@PSI)

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| --- | --- | --- | --- | --- | --- |
| Item | Example Implemented | Must HC | Should HC | Must UO | Nice UO |
| **Data Display** |  |  |  |  |  |
| live histogram display – X+Y vs. I | SNS/PSI | X |  |  |  |
| live histogram display – X/Y + λ/ToF vs. I | SNS/PSI | X |  |  |  |
| transformation of axes to Qz/pi-pf |  |  |  |  | X |
| save histogram images | SNS | X |  |  |  |
| way to compare histograms |  |  | X |  |  |
| selection, readout, cross-section of live display | SNS/PSI |  | X |  |  |
| ROI of histogram with integrated counts | SNS | X |  |  |  |
| full spin-state integration (one histogram for ++,--,+-,-+ with coupled ROI | SNS | X |  |  |  |
| λ-normalization by function and measured data |  | X |  |  | X |
| live binning and normalization to 1D-R(Q) |  |  | X | X |  |
| fast live counter of ROI/full detector for adjustment of instrument |  |  | X |  |  |
|  |  |  |  |  |  |
| **Under the Hood** |  |  |  |  |  |
| all relevant EPICS information saved in NeXuS |  | X |  |  |  |
| sample, user, experiment information in NeXuS |  | X |  |  |  |
| store experiment planning info (runs belonging to same reflectivity) |  |  | X | X |  |
|  |  |  |  |  |  |
| **Scripted Instrument Interface** |  |  |  |  |  |
| driving motors, setting limits, offsets |  | X |  |  |  |
| changing SEE parameters |  | X | X |  |  |
| reading SEE parameters |  | X |  |  |  |
| counting for time, monitor, counts, charge |  | X |  |  |  |
| counting for minimal statistic in R(Q) |  |  |  | X | X |
| simplified experiment planning (calculate slit sizes and angles for constant dQ/Q and desired overlap) | SNS/ILL |  | X | X |  |
| countinuous driving while counting (sweep) |  |  |  |  | X |
| loops, if-then |  | X |  |  |  |
| script simulation | MLZ |  |  | X |  |
| quick change of instrument setups (polarizer, SEE, detector distance) | SNS |  | X |  |  |
|  |  |  |  |  |  |
| **GUI Interface** |  |  | X | X |  |
| driving motors, setting limits, offsets |  | X | X |  |  |
| changing SEE parameters |  |  | X |  |  |
| reading SEE parameters |  |  | X |  |  |
| counting for time, monitor, counts, charge |  | X | X |  |  |
| counting for minimal statistic in R(Q) |  |  |  | X |  |
| simplified experiment planning (calculate slit sizes and angles for constant dQ/Q and desired overlap) |  |  |  | X |  |
| continuous driving while counting (sweep) |  |  |  |  | X |
| instrument calibration help (polarization calculation tools, low level commands, special plots e.g. alignment scans/ angle calibration etc.) | SNS | X |  | X |  |
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# Special instrument control

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| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Estia Selene guide segment alignment |  | X |  |  |  |
| Laser alignment and live feedback | PSI |  |  | X |  |
| Diverse alignment and interferometer support |  | X! |  |  | X |
| FREIA liquid height control feedback/interferometer | ILL, ISIS | X |  |  |  |
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# Data reduction general

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| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Full access to raw event data in Mantid and as NeXuS |  | X |  |  |  |
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# Data reduction conventional reflectometry (reference QuickNXS@SNS)

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| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Extract I(Q),I(λ) from I(X,Y,ToF) w/ XY-window | SNS | X |  |  |  |
| Normalize I(Q) by I(λ) of reference or direct beam => R(Q) | SNS | X |  |  |  |
| Subtract BG (const., c\*I(λ), ROI) | SNS | const. | X |  |  |
| Variable binning (const. dλ, dQ/Q) | SNS | X |  | X |  |
| Stitching support (foot print, fit overlap) | SNS | X |  |  |  |
| Angle from detector and pixel, allow overwrite | SNS | X |  |  |  |
| Full spin-state integration (same parameter for scaling and integration windows) ESTIA | SNS | X |  |  |  |
| Correct for bent samples | SNS |  |  | X |  |
| Live feedback during reduction (2D/1D/R) | SNS |  |  | X |  |
| Help algorithms (peak finder, parameter guesses) | SNS |  |  | X |  |
| Save to ASCII (Q, dQ, R, dR, alpha, lambda) | SNS | X |  |  |  |
| Automatic reduction mode | SNS |  | X | X | X |
| Reload reduction for reevaluation | SNS |  |  |  | X |
| Extract off-specular to R(Qz, pi-pf) / R(pi,pf) | SNS |  |  | X |  |
| smooth off-specular/interpolate to grid | SNS |  |  |  | X |
| filter/split events in run (SEE parameter, time, manual) |  |  |  |  | X |
| possible suppression of prompt pulse |  |  | X |  |  |
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# Data reduction high intensity specular reflectivity (reference amorreducer/eos@PSI)

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| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Extract 1D specular R(Q) from 3D dataset with proper normalization and footprint correction | PSI | X |  |  |  |
| Intermediate steps R(λ,θ), I(λ,θ) | PSI | X |  |  |  |
| Support functions to help analyze reduction |  |  |  |  | X |
| Live histogram of R(Q) with same algorithm |  |  |  |  | X |
| ASCII export of result and intermediates | PSI |  | X |  |  |
| Access of instrument scientist to reduction software sources |  | X |  |  |  |
| possible suppression of prompt pulse |  |  | X |  |  |
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# Data reduction GISANS (reference QuickNXS@SNS)

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| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Project event data on Qy, Qz, λ/Qx/pf | SNS |  |  |  | X |
| Histogram and normalize to 3D grid |  |  |  |  | X |
| Histogram and normalize to 2D grid in given λ-window | SNS |  |  |  | X |
| smooth data | SNS |  |  |  | X |
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# Cluster Simulation for Users

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| --- | --- | --- | --- | --- |
| Item | Must HC | Should HC | Must UO | Nice UO |
| BornAgain,  ~10-30 cores for simulations over few minutes fit of data can be much more expensive but low priority (1 night) |  |  |  | X |
| GenX,  ~1-30 cores for simulations and fits over few minutes fit of large datasets might reach hours |  |  | X |  |
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