Software requirements for Engineering Diffraction

(Reference instruments ENGIN-X@ISIS, Stress-Spec@FRMII, SALSA@ILL, Takumi@J-park)

HC = Hot Commissioning

UO = User Operations

# Main instrument control

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Example Implemented | Must HC | Should HC | Must UO | Nice UO |
| **Data Display** |  |  |  |  |  |
| 2D (live) raw counts data for each detector (possibility change axis between λ, 2θ, ToF, d, Q) | Stress-Spec, ENGIN-X, SALSA | X |  |  |  |
| 1D (live) histogram display: integrated intensity over all detector area vs ToF (λ, d, Q) (for each detector) | Stress-Spec, Takumi | X |  |  |  |
| 1D (live) histogram of ROI with integrated counts vs ToF (λ, d, Q, 2θ) | Takumi |  | X |  |  |
| Correction of the (live) detector data for distortions, efficiency, calibration |  |  | X |  |  |
| Incident beam spectrum |  | X |  |  |  |
| Plot of SE parameters (temp, stress, position, etc.) as a function of time | Stress-Spec, ENGIN-X | X |  |  |  |
| Visualization of the positioning system status |  |  | X |  |  |
| Transformation of engineering SE parameters to strain, stress, etc. | Stress-Spec, ENGIN-X, SALSA, Takumi | X |  |  |  |
| Way to compare histograms (fix display of pattern in specific state to see current change) |  | X |  |  |  |
| Save detector and 1D histogram images |  | X |  |  |  |
| Region of interest (ROI) selection  |  | X |  |  |  |
| Remote access to (live) data  |  | X |  |  |  |
| Remote access to instrument status, incl. notification in case of failures |  | X |  |  |  |
| Selection of relevant Data |  | X |  |  |  |
| … |  |  |  |  |  |
| **Under the Hood** |  | X |  |  |  |
| All relevant EPICS information saved in NeXuS |  | X |  |  |  |
| Selection of relevant parameters |  |  |  |  |  |
| Sample, user, experiment information in NeXuS |  | X |  |  |  |
| Logbook of entire experiment including instrument configuration, beam status and SEE parameters |  | X |  |  |  |
|  |  |  |  |  |  |
|  |  |  |  |  |  |
| **Scripted Instrument Interface** |  |  |  |  |  |
| Driving motors, setting limits, offsets |  | X |  |  |  |
| Changing SEE parameters |  | X |  |  |  |
| Reading SEE parameters |  | X |  |  |  |
| Counting for time, monitor, counts, charge |  | X |  |  |  |
| Simplified experiment planning  |  | X |  |  |  |
| Continuous driving while counting (sweep) |  | X |  |  |  |
| Loops, if-then |  | X |  |  |  |
| sequences |  | X |  |  |  |
| Script simulation, check for failure/logic |  | X |  |  |  |
| Quick change of instrument setups (SE, high/low resolutions, multiplexing) |  | X |  |  |  |
|  |  |  |  |  |  |
| **GUI Interface** |  |  |  |  |  |
| Driving motors, setting limits, offsets |  |  | X |  |  |
| Changing SEE parameters |  |  | X |  |  |
| Reading SEE parameters |  |  | X |  |  |
| Counting for time, monitor, counts, charge |  |  | X |  |  |
| Read of pre-measured 3D coordinates and scanning path planning (ex. SScanSS) | ENGIN-X |  | X |  |  |
| Adjustment and visualization of positioning system (hexapod, robot, tables, etc.) |  |  |  | X |  |
| Quick change of instrument setups (SE, high/low resolutions, multiplexing) |  |  |  | X |  |
| Simplified experiment planning (experiment tree structure) |  |  | X |  |  |
| Experiment simulation for multiplexing (predict overlap, adjust the MC speed) |  |  |  | X |  |
| Continuous driving while counting (sweep) |  |  | X |  |  |
|  |  |  |  |  |  |
| **Instrument Live feedback** |  |  |  |  |  |
| Choppers frequency and position (measurement mode) |  | X |  |  |  |
| Beam power monitor | Stress-Spec, SALSA | X |  |  |  |
| SEE parameters | Stress-Spec | X |  |  |  |
| Sample position status | Stress-Spec | X |  |  |  |

# Special instrument control

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Laser/Optical alignment of sample positions |  | X |  |  |  |
| SE calibration procedure (deformation rig) |  | X |  |  |  |
| Simple real-time data analysis (individual peak fitting) with active feedback to control SE |  |  |  | X |  |
| SSCANSS or related sample positioning system |  |  | X | X |  |
| Tomography or CAD model driven diffraction (implemented in sample positioning system) |  |  |  | x |  |
| Drivers for SE (integration into EPICS) |  | X |  |  |  |
| Integrate complementary characterization tools into data stream (maybe even use for control feedback): strain gauges, extensometers, digital Image Correlation, Acoustic Emission tests (Note: Some of these are currently developed in the CZ-ESS OP project) |  |  |  |  |  |
|  |  |  |  |  |  |

# Data reduction general

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Full access to raw events data in Mantid and as NeXuS |  | X |  |  |  |
| Full access to SE and instrument status tags events data in Mantid and as NeXuS |  | X |  |  |  |
| Multiplex data reductions |  | X |  |  |  |

# Data reduction conventional engineering

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Correction for detector distortions, efficiency, calibration |  | X |  |  |  |
| Correction for detector discrimination, amplification, … |  | X |  |  |  |
| Automated check and adaption of detector discrimination |  | X |  |  |  |
| Normalization of events to incident beam |  | X |  |  |  |
| Background subtraction |  |  | X |  |  |
| Variable binning (SE parameters, time, ToF, Q, d, manual) |  | X |  |  |  |
| Extraction of 0D (integrated intensity) |  | X |  |  |  |
| Extraction of 1D I(Q), I(d), I(ToF/sin) |  | X |  |  |  |
| Extraction of 2D I(ToF, 2θ), I(ToF/sin, sin) I(ToF, d) |  | X |  |  |  |
| Help algorithms (peak finder, prediction of relevant peaks – sample information) |  | X |  |  |  |
| Automatic reduction mode |  |  |  | X |  |
| Reload reduction for reevaluation |  | X |  |  |  |
| Save to ASCII (Q, I, FWHM, Dd/d, ToF-d matrix) |  | X |  |  |  |

# Data reduction special engineering

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| Extraction of reference d for multiplexing technique (guess based on sample information, manual) |  | X |  |  |  |

# Data acquisition and storage

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Item | Already Implemented | Must HC | Should HC | Must UO | Nice UO |
| **Data Acquisition Parameters** |  |  |  |  |  |
| Time (Global Clock) |  | X |  |  |  |
| Proton Pulse |  | X |  |  |  |
| Chopper disks position |  | X |  |  |  |
| Beam Monitor  |  | X |  |  |  |
| Detectors  |  | X |  |  |  |
| Slit position (opening) |  | X |  |  |  |
| Motor axis positions |  | X |  |  |  |
|  |  |  |  |  |  |
| **SEE parameters** |  |  |  |  |  |
| Temperature |  | X |  |  |  |
| Load |  | X |  |  |  |
| Motor position |  | X |  |  |  |
| Vacuum |  |  | X |  |  |
|  |  |  |  |  |  |
| **Special requirements** |  |  |  |  |  |
| Off-beam SEE parameters for long term experiments (stand-alone mode) |  | X |  |  |  |
|  |  |  |  |  |  |
| **Data storage** |  |  |  |  |  |
| Max. data rate of detectorsat max. global intensity i.e\*  | 550 MB/s |  |  |  |  |
| Average data rate | 3 MB/s |  |  |  |  |
| Average events/s | 3 x105  |  |  |  |  |
| Average time per experiment | Few min. to several h |  |  |  |  |
|  |  |  |  |  |  |
| **Data format** |  |  |  |  |  |
| ASCII |  | X |  |  |  |
| HTML5 |  |  |  |  | X |
| NEXUS |  | X |  |  |  |
| …… |  |  |  |  |  |
|  |  |  |  |  |  |
| **Data analysis** |  |  |  |  |  |
| Single peak fitting (FWHM, peak position, intensity) |  | X |  |  |  |
| Full pattern fitting (FWHM, peak position, intensity) |  | X |  |  |  |
| Rietveld refinement |  | X |  |  |  |
| Texture |  |  |  |  |  |
|  |  |  |  |  |  |
| **Data analysis tools** |  |  |  |  |  |
| MAUD |  |  |  |  |  |
| FullProf |  |  |  |  |  |
| GSAS 2 |  |  |  |  |  |
|  |  |  |  |  |  |
| **Modelling** |  |  |  |  |  |
| Needs and requirements are to still to be collected  |  |  |  |  |  |
| Correct signal for beam attenuation (especially in complex geometries) |  |  |  |  |  |
| Access to FEM software  |  |  |  |  |  |

\*(1 MHz count rate on 1m2 active area @ 2 m sample detector distance)