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			
…					
Under the Hood		X			
All relevant EPICS information saved in NeXuS		X			
Sample, user, experiment information in NeXuS		X			
Logbook of entire experiment including instrument configuration, beam status and SEE		X			

parameters					
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			
Script simulation		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	

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			
Normalization of each event to incident beam		X			
Background subtraction			X		
Variable binning (SE parameters, time, ToF, Q, d, manual)		X			
Extraction of 1D I(Q), I(d)		X			
Extraction of 2D I(ToF, 2θ), 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 d_0 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 detectors (day 1)	550 Mb/s				
Data format					
ASCII		X			
HTML5					X
NEXUS		X			