BornAgain functionality for reflectometry

	Item	DEMO	GUI	Python (script)	Notes	
Reflectivity Data/Plot/IO						
	Simulate and plot single curve/channel/contrast	reflectometry	yes	yes		
	Simulate and fit multiple		no	yes	The same model with varying contrasts (including X-ray) and associated constraints	
	Read ASCII data in program defined format		yes	yes		
	Read different ASCII format (column order)		no	yes	Ongoing work on the dedicated loader but not in the current release.	
	theta/tth as x-axis		no	no	BornAgain reads in https://genx.sourceforge.io/doc/_downloads/xray-tutorial.dat, which is tth but doesn't change unit axis label	
	q as x-axis		yes	yes	Qz as x-axis is available for plot representation and data loading both in GUI and the core. Units switch is indeed not possible.	
	RQ^4 (or RQ^2) as y-axis		no	yes	Example Implementation: Motofit/Refnx	
	R/Rf as y-axis		no	no	Example Implementation: Motofit/Refnx	
	Read and use resolution column from file	tof-with-resolution	no	yes	Resolution can be specified as a vector of values. Reading must be performed with built-in python tools (e.g. numpy.load). In the example, there is no reading phase, but one can see how to specify a vector of dq's. Both relative and absolute resolutions are available	
	Simulate at data points		yes	yes		
	Simulate arbitrary q/tth-points (e.g. ToF)	time-of-flight	no	yes		
	Plot data with simulation		yes	yes		
	Plot multiple datasets with		no	no		

	simulations					
	Publication quality graphs		no	no	Nice plots can be made but may require some intuitive setup of resolution	
	Export simulated data as ASCII		yes	yes		
	Scaling, calculation on data columns		no	yes	Ongoing work on the dedicated data loader but not available from current release.	
	Instrument specific import filters (templates/plugins)		no	no	Example Implementation: GenX	
	Batch processing of fits for multiple datasets		no	yes	Example Implementation: Refnx	
Other Visualizations						
	SLD profile	material-profile	no	yes		
	SLD profile with embedded particles	material-profile-with-particles	no	yes		
	Magnetic SLD profile		no	no	Example Implementation: GenX	
	Integrate magnetic moment		no	no		
	Figure of Merit (FOM) vs. iteration		yes	yes	Example Implementation: GenX	
	Scan of parameter vs. FOM		no	no	Example Implementation: GenX	
	Calculate/Show spin-asymmetry		no	no		
	Total reflection = unity (i.e. y axis is R not I)		no	yes		
Sample Model						
	Layer roughness analytical	specular-simulation-with-roughness	yes	yes		
	Layer roughness by sub-division		no	yes		

	Material by refractive index		yes	yes		
	Material by SLD	material types	yes	yes	Includes complex-valued SLD (inv. squared Angstroms units only)	
	Material by mixure of SLD (deuteration)		no	yes	Example Implementation: RasCAL	
	Material by Formula and density		no	yes	Example Implementation: GenX, Refnx/Motofit	
	Material by Formula or molecular scattering length + molecular volume		no	yes	Example Implementation: GenX, Refnx/Motofit	
	Database for materials (manual or online)/ SLD calculator		no	yes	Ongoing work on GUI. Example Implementation: GenX,online, Refnx/Motofit	
	Include solvation (mixing of the layer SLD with the solvent SLD)		no	no	Example Implementation: Refnx/Motofit	
	Analytic function for SLD(z)		no	no		
	SLD calculator proteins		no	no		
	Repeating structures		no	yes		
	Magnetization surface density of sample		no	no		
	Angle of magnetization to polarization		no	no		
	Wavelength dependent absorption (resonances)		no	no		
	Layer model editor		no	N/A	Mock-up available to be integrated in the next release	
Instrument/Physical effects						
	Footprint correction (square beam)	footprint-correction	yes	yes		
	Footprint correction (Gaussian or		yes (guassian	yes (guassian	Example Implementation: GenX	

	other shape)		& square)	& square)		
	Beam angular spread (constant)	beam-angular-divergence	yes	yes	One parameter	
	Beam wavelength spread (constant)	beam-full-divergence	yes	yes		
	Proper resolution treatment for ToF (angular+WL)	time-of-flight and tofr-with-resolution	no	no	Resolution can be specified only in the units used for instrument definition. Thus if a qz-range is specified for the instrument, resolution must be specified as dqz. Example Implementation: GenX (script)	
	Arbitrary spread on x-axis		yes	yes		
	Polarization		no	yes		
	Polarization Analysis		no	yes	Recently implemented in develop version for neutrons only. Further work on cross-validation is required. Seemingly easily transferable to GUI.	
	X-ray energy dependence		no	no	Example Implementation: GenX	
	Constant background		yes	yes	In GUI this is part of instrument setup but potentially this should be done per data set?	
	Scaling of intensity		no	no		
Refinement						
	Gradient decent refinement log (+ errors)		no	yes	No for GUI due to lack of uncertainty treatment	
	Gradient decent refinement chi² + errors	fit-with-uncertainties	no	yes	No for GUI due to lack of uncertainty treatment	
	Genetic/Global refinement	fit-specular-data	yes	yes		
	Choice of minimisation algorithm		yes	yes	Genetic, Levenberg-Marquardt or other least-squares, MCMC	
	User defined FOM		no	yes	Example Implementation: GenX (script)	
	Co-refinement multiple datasets including pol/contrasts		no	yes	Example Implementation: GenX	

	Co-refinement x-ray/neutron		no	yes		
	Same sample parameters for multiple probes (x-ray/neutron up/neutron down/...) and possible specification of few changing parameters (magnetization/deuteration per dataset)		no	no	Example Implementation: GenX	
	Adjust weighting of co-refined datasets (e.g. x-ray vs. neutron)		no	yes		
	Direct parameter constraints (equal)		yes	yes		
	Indirect parameter constraints (function of others)		no	yes	Example Implementation: GenX	
	Apply arbitrary mathematical constraints between variables within a model (over different contrasts)		no	no	Example Implementation: RasCal/Refnx	
	Parameter fit ranges (min/max)		yes	yes		
	Evaluation of parameter uncertainties (from Chi^2)		no	yes	It can be accomplished with some of the ROOT minimizers used.	
	Baysean Analysis for model comparison and parameter correlations		no	no		
	Integration of advanced/scripted model into GUI		yes	N/A	Currently available for importing the sample structure.	
Community outreach						
	Interoperable software so it can be integrated with other tools				This is a soft requirement, which for example involves collaboration with ORSO https://reflectivity.github.io/.	