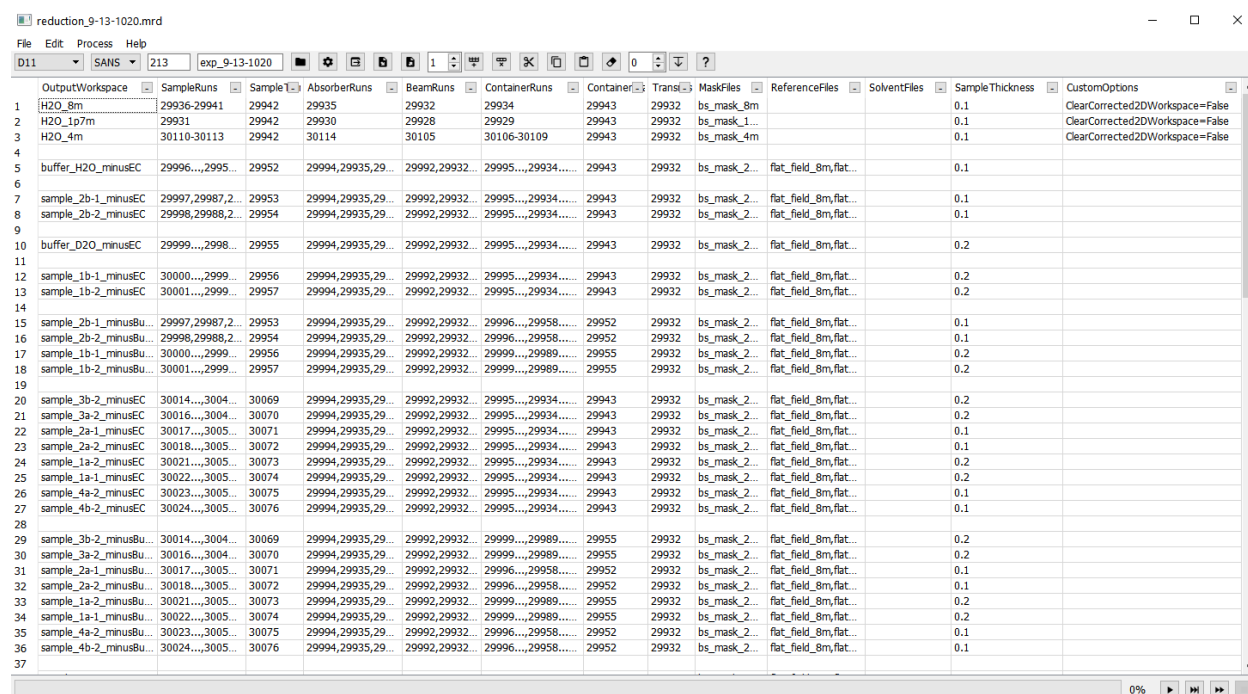


Mantid user interfaces at ILL

The only “special” interface that we are planning to use/develop is DrILL (see <https://docs.mantidproject.org/nightly/interfaces/ILL/DrILL.html>)

Basically it is just a spreadsheet serving as an interface to the ILL AutoProcess algorithms, which perform the full data reduction. Thus instead of calling repeatedly the AutoProcess algorithm or writing a python script to do it, the user fills an “excel-like” table like this:



	OutputWorkspace	SampleRuns	Sample	AbsorberRuns	BeamRuns	ContainerRuns	Trans	MaskFiles	ReferenceFiles	SolventFiles	SampleThickness	CustomOptions
1	H2O_8m	29936-29941	29942	29935	29932	29934	29943	29932	bs_mask_8m		0.1	ClearCorrected2DWorkspace=False
2	H2O_1p7m	29931	29942	29930	29928	29929	29943	29932	bs_mask_1...		0.1	ClearCorrected2DWorkspace=False
3	H2O_4m	30110-30113	29942	30114	30105	30106-30109	29943	29932	bs_mask_4m		0.1	ClearCorrected2DWorkspace=False
4												
5	buffer_H2O_minusEC	29996...,2995...	29952	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
6												
7	sample_2b-1_minusEC	29997,29987,2...	29953	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
8	sample_2b-2_minusEC	29998,29988,2...	29954	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
9												
10	buffer_D2O_minusEC	29999...,2998...	29955	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
11												
12	sample_1b-1_minusEC	30000...,2999...	29956	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
13	sample_1b-2_minusEC	30001...,2999...	29957	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
14												
15	sample_2b-1_minusEC	29997,29987,2...	29953	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
16	sample_2b-2_minusEC	29998,29988,2...	29954	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
17	sample_1b-1_minusEC	30000...,2999...	29956	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
18	sample_1b-2_minusEC	30001...,2999...	29957	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
19												
20	sample_3b-2_minusEC	30014...,3004...	30069	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
21	sample_3a-2_minusEC	30016...,3004...	30070	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
22	sample_2a-1_minusEC	30017...,3005...	30071	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
23	sample_2a-2_minusEC	30018...,3005...	30072	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
24	sample_1a-2_minusEC	30021...,3005...	30073	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
25	sample_1a-1_minusEC	30022...,3005...	30074	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
26	sample_4a-2_minusEC	30023...,3005...	30075	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
27	sample_4b-2_minusEC	30024...,3005...	30076	29994,29935,29...	29992,29932...	29995...,29934.....	29943	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
28												
29	sample_3b-2_minusEC	30014...,3004...	30069	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
30	sample_3a-2_minusEC	30016...,3004...	30070	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
31	sample_2a-1_minusEC	30017...,3005...	30071	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
32	sample_2a-2_minusEC	30018...,3005...	30072	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
33	sample_1a-2_minusEC	30021...,3005...	30073	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
34	sample_1a-1_minusEC	30022...,3005...	30074	29994,29935,29...	29992,29932...	29999...,29989.....	29955	29932	bs_mask_2...	flat_field_8m,flat...	0.2	
35	sample_4a-2_minusEC	30023...,3005...	30075	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
36	sample_4b-2_minusEC	30024...,3005...	30076	29994,29935,29...	29992,29932...	29996...,29958.....	29952	29932	bs_mask_2...	flat_field_8m,flat...	0.1	
37												

Aims:

1. Present a global view of a whole experiment in a single table showing the run numbers and main files used in the reduction.
2. Hide the complexities of the equivalent script needed to repeat the same treatment for hundreds of samples for some users who are not comfortable with python.

Limitations:

1. No visualization. Final results are saved as Mantid workspaces and as files (NeXus or Ascii), so in order to see them the user needs to go back to the workbench and use the standard tools provided by Mantid (show instrument / slice viewer / plot /superplot), depending on the type of data.
2. No customized / responsive interface (e.g. Grasp-like for those who know Grasp). The settings interface appears as a list of all the available input parameters and the reduction is run using those. If the user decides to change something, he/she needs to modify the needed values and run again the full table or the selected rows.

The columns available and their names depend on the technique/instrument, and they can be customized (removed from the table if not needed, contracted/expanded, etc.). Each row corresponds to one sample (in the SANS example above each sample is measured at 3 different detector distances and all of them are reduced in a single call to SANSILLAutoProcess). Global settings to be applied to each of the rows are defined in the menu:

Parameter	Value
ThetaDependent	<input checked="" type="checkbox"/>
SensitivityMaps	
DefaultMaskFile	edge_mask_8m
NormaliseBy	Monitor
SampleThickness	0.1
TransmissionBeamRadius	0.1
BeamRadius	0.1
WaterCrossSection	1.0
MaxQxy	-1.0
DeltaQ	-1.0
OutputPanels	<input type="checkbox"/>
OutputType	I(Qx,Qy)
CalculateResolution	DirectBeam
DefaultQBinning	PixelSizeBased
BinningFactor	1.0
NPixelDivision	1
NumberOfWedges	0
WedgeAngle	30.0
WedgeOffset	0.0
AsymmetricWedges	<input type="checkbox"/>
IQxQyLogBinning	<input type="checkbox"/>
WavelengthRange	1.0,10.0
OutputBinning	
ClearCorrected2DWorkspace	<input checked="" type="checkbox"/>
StitchReferenceIndex	1
ShapeTable	
Wavelength	0.0

“Special” rows needing different parameters can be reduced in the same table by changing those global parameters using the CustomOptions column.

Samples that share some of the inputs (e.g. same background) can be grouped together, so the needed information is written only for the first sample in the group:

mantid_all_9-13-1033.mrd

File Edit Process Help

D11 SANS 213 exp_9-13-1033

	OutputWorkspace	SampleRuns	SampleTransmissionRuns	AbsorberRuns	BeamRuns	ContainerRuns	ContainerTransmissionRuns	TransmissionBeamRuns	MaskFiles	ReferenceFiles	SampleThickness
1	H2O_01p7m	19758	19761	19760	19756	19759	19762	19763	bs_mask_02m		0.1
2	H2O_08m	19764	19761	19766	19763	19765	19762	19763	bs_mask_08m		0.1
3											
A1	EO-DMA-d15 pH7.5 D...	19793...,1979...	19787	19768,19766,19...	19769,19763...	19767,19765,197...	19762	19763	bs_mask_3...	flat_field_08m,fla...	0.1
A2	EO-DMA pH7.5 D2O	19794...,1979...	19788								
A3	D2O_50mM NaCl	19795,19792,1...	19789								
A4	EO-DMA 5gL-ins 2.5g...	19800,19811,1...	19809								
A5	H2O-D2O 65-35	19801,19812,1...	19810								
A6	EO-DMA 5gL-ins 1gL...	19874,19844,1...	19829								
A7	EO-DMA 5gL-ins 2.5g...	19875,19845,1...	19830								
A8	ins 1gL D2O	19876...,1984...	19831								
A9	ins 2.5gL D2O	19877,19847,1...	19832								
A10	EO-DMA-d16 5gL-ins ...	19878,19848,1...	19833								
A11	EO-DMA-d15 5gL-ins ...	19879,19849,1...	19834								
A12	myo 2.5gL D2O	19880,19850,1...	19835								
A13	EO-DMA 5gL-myo 2.5...	19881,19851,1...	19836								
A14	EO-DMA-d15 5gL-myo...	19882,19852,1...	19837								
A15	EO-DMA 1gL pH 7.5 ...	19883,19853,1...	19838								
A16	EO-DMA 1gL-ins 0.5g...	19884,19854,1...	19839								
A17	EO-DMA 5gL-ins 1gL...	19885,19855,1...	19840								
A18	EO-DMA 5gL-myo 1gL...	19886,19856,1...	19841								
A19	EO-DMA-d15 5gL-myo...	19887,19857,1...	19842								
A20	EO-DMA 5gL pH7.5 H...	19888,19858,1...	19843								
24											
B1	EO-DMA 5gL-ins 2.5g...	19800,19811,1...	19809	19768,19766,19...	19769,19763...	19801,19812,198...	19810	19763	bs_mask_3...	flat_field_08m,fla...	0.1
B2	EO-DMA 5gL-ins 1gL...	19885,19855,1...	19840								
B3	EO-DMA 5gL pH7.5 H...	19888,19858,1...	19843								
28											
C1	EO-DMA-d15 pH7.5 D...	19793...,1979...	19787	19768,19766,19...	19769,19763...	19795,19792,197...	19789	19763	bs_mask_3...	flat_field_08m,fla...	0.1
C2	EO-DMA pH7.5 D2O...	19794...,1979...	19788								
C3	EO-DMA 5gL-ins 1gL...	19874,19844,1...	19829								
C4	EO-DMA 5gL-ins 2.5g...	19875,19845,1...	19830								
C5	ins 1gL D2O_minus_D...	19876...,1984...	19831								
C6	ins 2.5gL D2O_minus...	19877,19847,1...	19832								
C7	EO-DMA-d16 5gL-ins ...	19878,19848,1...	19833								
C8	EO-DMA-d15 5gL-ins ...	19879,19849,1...	19834								

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We are currently working in creating a second table associated to this one, where the parameters of each group are displayed and can be modified:

mantid_all_9-13-1033.mrd

File Edit Process Help

D11 SANS v1 Cycle Experiment

	OutputWorkspace	SampleRuns	SampleTransmissionRuns	AbsorberRuns	BeamRuns	ContainerRuns	ContainerTransmissionRuns
1	H2O_01p7m	19758	19761	19760	19756	19759	19762
2	H2O_08m	19764	19761	19766	19763	19765	19762
3							
A1	EO-DMA-d15 pH7...	19793...,197...	19787				
A2	EO-DMA pH7.5 D2O	19794...,197...	19788				
A3	D2O_50mM NaCl	19795,1979...	19789				
A4	EO-DMA 5gL-ins 2...	19800,1981...	19809				
A5	H2O-D2O 65-35	19801,1981...	19810				
A6	EO-DMA 5gL-ins						
A7	EO-DMA 5gL-ins						
A8	ins 1gL D2O						
A9	ins 2.5gL D2O						
A10	EO-DMA-d16 5gL...						
A11	EO-DMA-d15 5gL...						
A12	myo 2.5gL D2O						
A13	EO-DMA 5gL-myo						
A14	EO-DMA-d15 5gL...	19882,1985...	19837				
A15	EO-DMA 1gL pH 7...	19883,1985...	19838				
A16	EO-DMA 1gL-ins 0...	19884,1985...	19839				
A17	EO-DMA 5gL-ins 1g...	19885,1985...	19840				
A18	EO-DMA 5gL-myo ...	19886,1985...	19841				
A19	EO-DMA-d15 5gL...	19887,1985...	19842				
A20	EO-DMA 5gL pH7.5...	19888,1985...	19843				
24							
B1	EO-DMA 5gL-ins 2...	19800,1981...	19809				
B2	EO-DMA 5gL-ins 1g...	19885,1985...	19840				
B3	EO-DMA 5gL pH7.5...	19888,1985...	19843				

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Group settings

	AbsorberRuns	BeamRuns	ContainerRuns	ContainerTransmissionRuns
A	19768,19766,19760	19769,19763,19756	19767,19765,19759	19762
B	19768,19766,19760	19769,19763,19756	19801,19812,19808	19810
C	19768,19766,19760	19769,19763,19756	19795,19792,19786	19789

OK Cancel