User interfaces

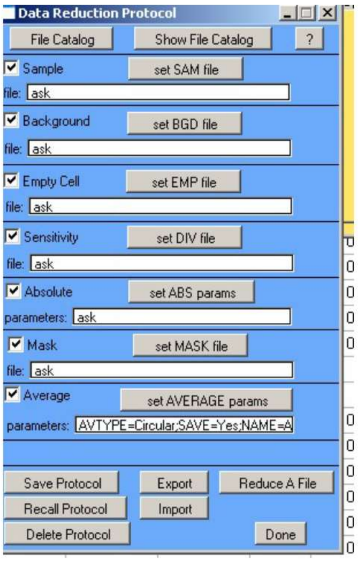
ILL

See separate file

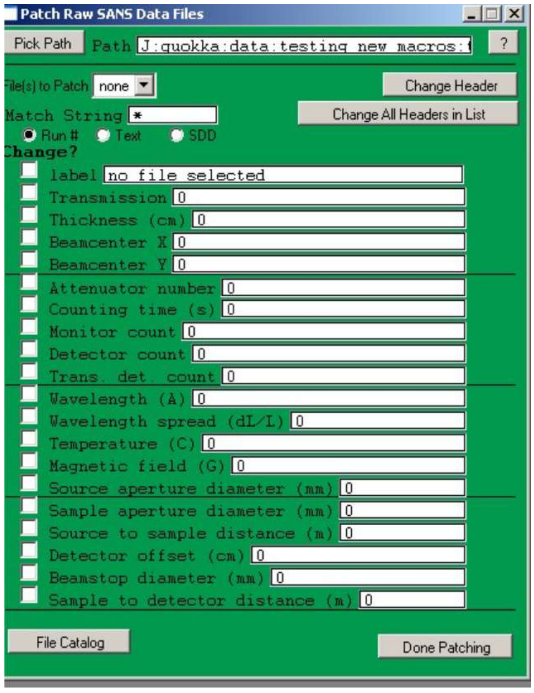
ANSTO, Quokka SANS

NIST macros

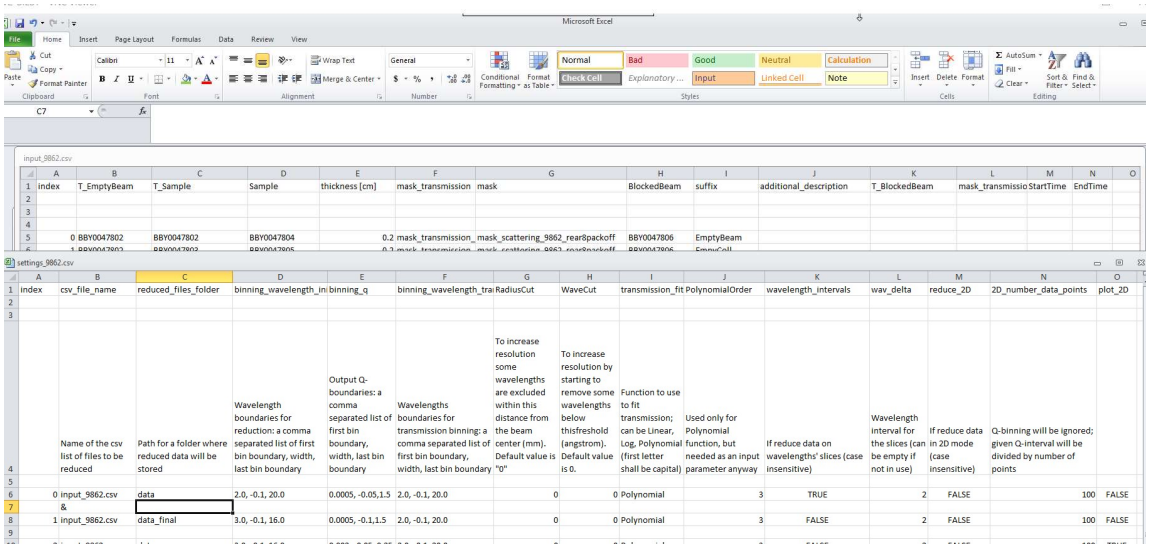
https://www.ansto.gov.au/sites/default/files/2022-03/QUOKKA%20user%20manual%20March%202022.pdf



Leaving 'ask' will mean that during the reduction Igor will prompt you to select the file you wish to use:



ANSTO Bilby SANS, no GUI, files & reduction are kept in the csv files:



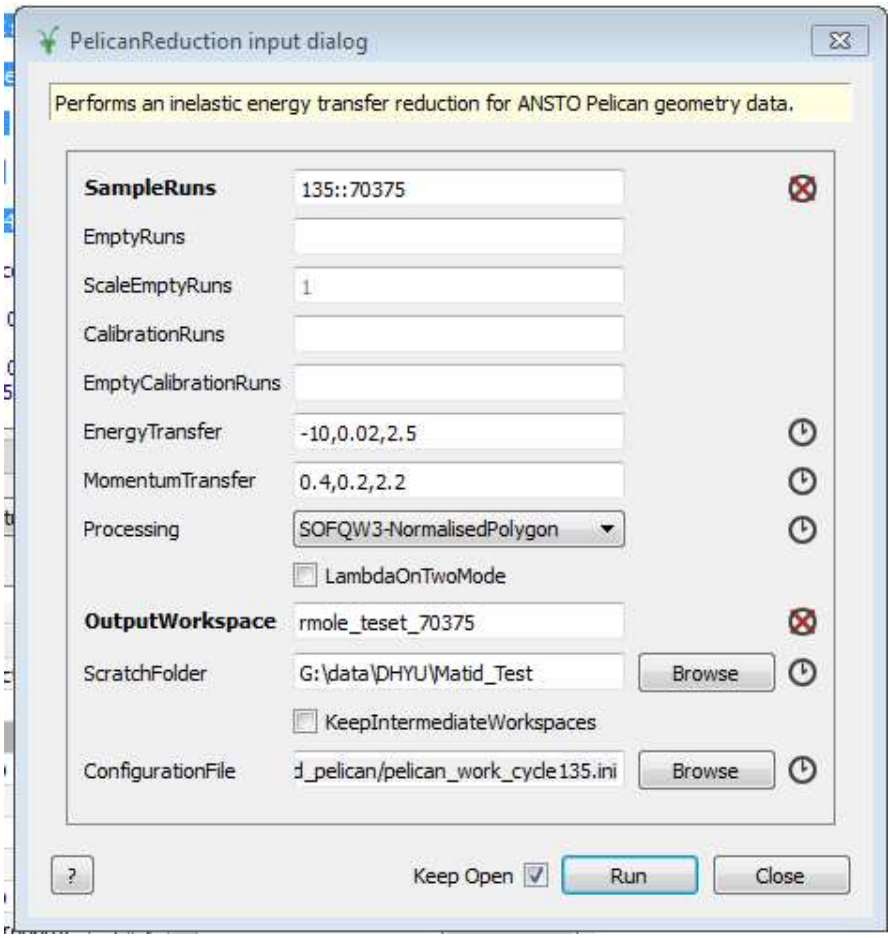
input_9862.csv

index	T_EmptyBeam	T_Sample	Sample	thickness [cm]	mask_transmission	mask	BlockedBeam	suffix	additional_description	T_BlockedBeam	mask_transmissio	StartTime	EndTime
0	BBY0047802	BBY0047802	BBY0047804	0.2	mask_transmission_	mask_scattering_9862_rear8packoff	BBY0047806	EmptyBeam					

settings_9862.csv

index	csv_file_name	reduced_files_folder	binning_wavelength_in	binning_q	binning_wavelength_tra	RadiusCut	WaveCut	transmission_fit	PolynomialOrder	wavelength_intervals	wav_delta	reduce_2D	2D_number_data_points	plot_2D
	Name of the csv list of files to be reduced	Path for a folder where reduced data will be stored	Wavelength boundaries for reduction: a comma separated list of first bin boundary, width, last bin boundary	Output Q-boundaries: a comma separated list of first bin boundary, width, last bin boundary	Wavelengths boundaries for transmission binning: a comma separated list of first bin boundary, width, last bin boundary	To increase resolution some wavelengths are excluded within this distance from the beam center (mm). Default value is "0"	To increase resolution by starting to remove some wavelengths below thisfreshold (angstrom). Default value is 0.	Function to use to fit transmission; can be Linear, Log, Polynomial (first letter shall be capital)	Used only for Polynomial function, but needed as an input parameter anyway	If reduce data on wavelengths' slices (case insensitive)	Wavelength interval for the slices (can be empty if not in use)	If reduce data in 2D mode (case insensitive)	Q-binning will be ignored; given Q-interval will be divided by number of points	
0	input_9862.csv	data	2.0, -0.1, 20.0	0.0005, -0.05,1.5	2.0, -0.1, 20.0	0	0	Polynomial	3	TRUE	2	FALSE	100	FALSE
1	input_9862.csv	data_final	3.0, -0.1, 16.0	0.0005, -0.1,1.5	2.0, -0.1, 20.0	0	0	Polynomial	3	FALSE	2	FALSE	100	FALSE

ANSTO ToF spectrometer Pelican (this is the current state, shall be improved) (to note: backscattering Emu has similar User interface; Emu reduction code is still not in the release):



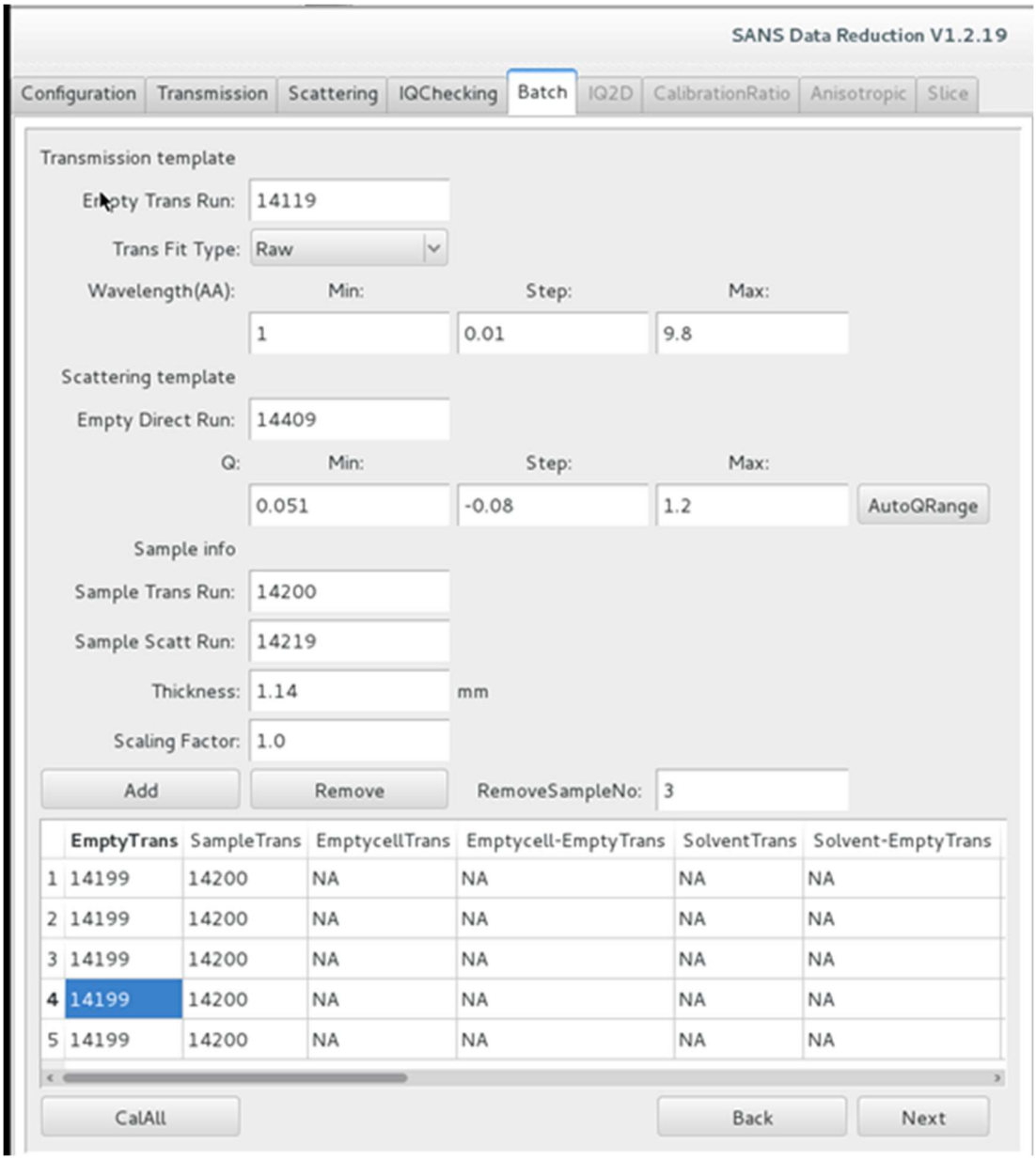
There is a QENS fitting tool that ISIS developed for Mantid that seems very useful that we are only just starting to use.

I also want to learn about the VATES option for single crystal processing (as currently we split this into two and start with Mantid, but finish with Horace/matlab).

CSNS

The attached figure is the batch processing interface we use currently. RunNo for each sample and its transmission and EB/EC need to be type in manually, and by clicking add button, these information will be stored in the spreadsheet on the bottom, and can be edited in the spreadsheet later. By clicking the CalAll button, every entry in the spreadsheet will be calculated sequentially.

We are hoping that the Batch processing interface could allow the upload of an excel or cvs file, from where the relevant run number and other information for each sample can be extracted directly.



GISANS

ISIS

The GISANS is not in the priority list of the Large Scale Structure group so won't get done for a while so anything that has been done already and could be expanded in a collaborative way would be great.

CSNS

In terms of GISANS, we hope Mantid could provide a specified GISANS data visualization interface similar to the current Instrument interface. We hope the interface would allow us to bin the data within certain wavelength range and make line cuts in vertical and horizontal directions and obtain and store the intensity distribution along the line (like imageJ).
The transmission correction for GISANS data has always been a problem for us as spallation neutron source. I am not sure if I could count on Mantid to solve this issue though. I would be grateful if we could discuss this issue in the further discussion

ANSTO

I've talk to our scientist from our second SANS machine, they have GISANS set-up. For the data, they've used Grasp, just to get an integrated intensity across a chosen area of detectors. And I cannot see a wish to put an effort into the Mantid GISANS part.

Algorithms that need improvements and validation tests

- Pascal Manuel:

Absorption corrections

- Anna Sokolova:

wide_angle_correction
(https://docs.mantidproject.org/nightly/algorithms/SANSWideAngleCorrection-v1.html).