SAS 2024

CanSAS: data reduction

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Bilby SANS (Andrew Whitten, Liliana de Campo)

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ANSTO

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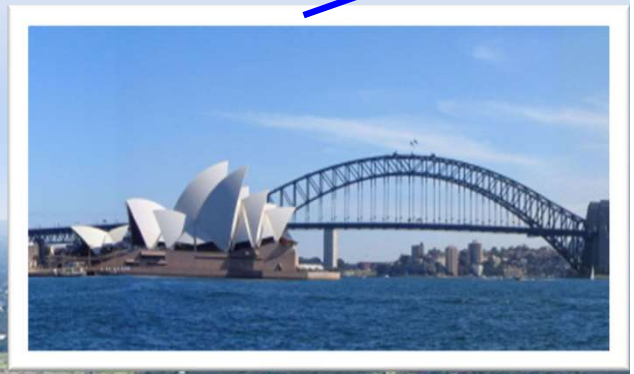
Science. Ingenuity. Sustainability.

ANSTO Lucas Heights Campus & OPAL Reactor

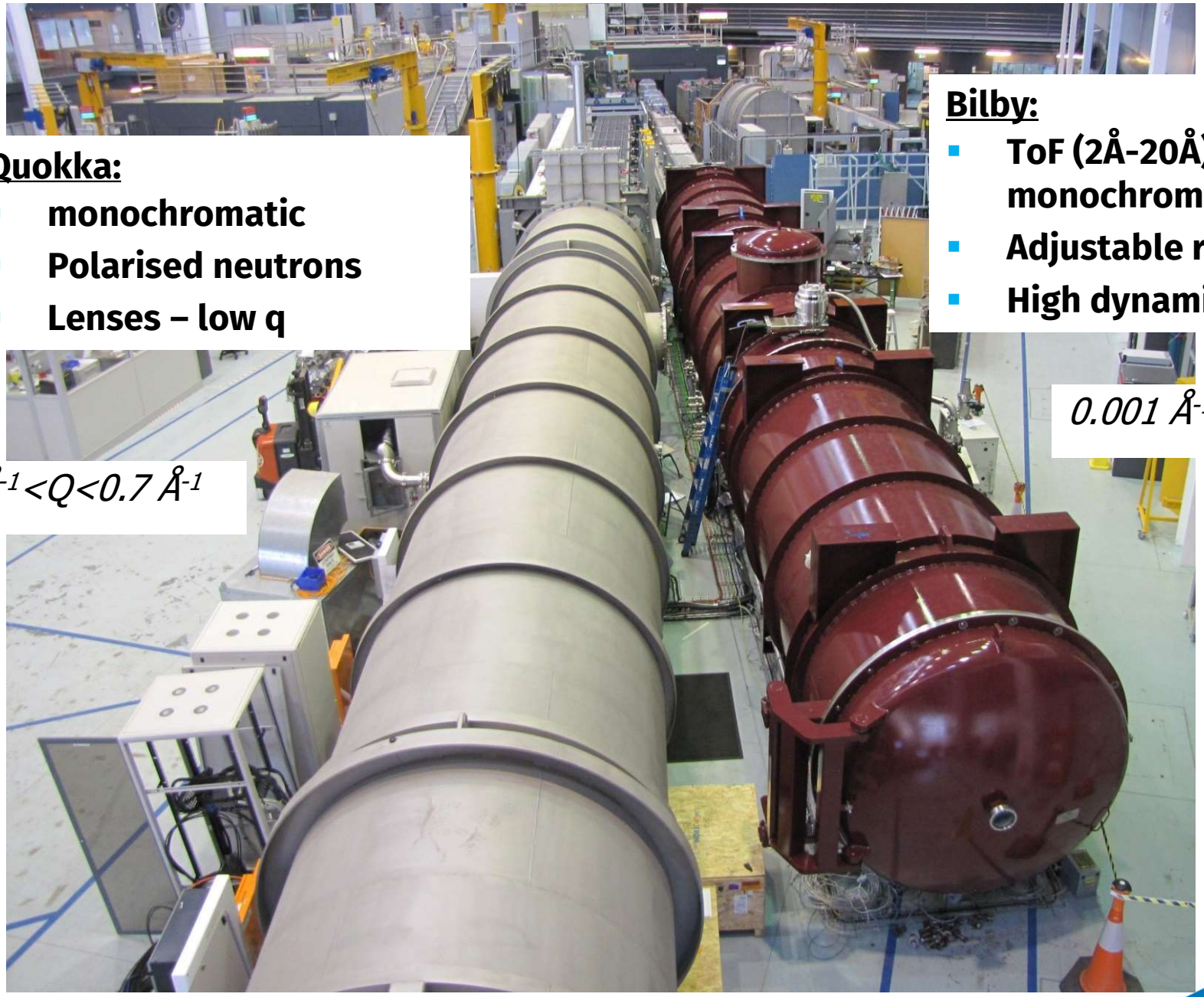
- 20 MW
- Open pool
- Compact core

- D_2O reflector
- Plate type Low Enriched Uranium fuel
- Commenced operation 2006



OPAL

SANS at ACNS: Bilby & Quokka



Quokka:

- monochromatic
- Polarised neutrons
- Lenses – low q

0.0007 Å^{-1}<Q<0.7 Å^{-1}

Bilby:

- ToF (2Å-20Å) and/or monochromatic
- Adjustable resolution
- High dynamic q range

0.001 Å^{-1}<Q<1.8 Å^{-1}

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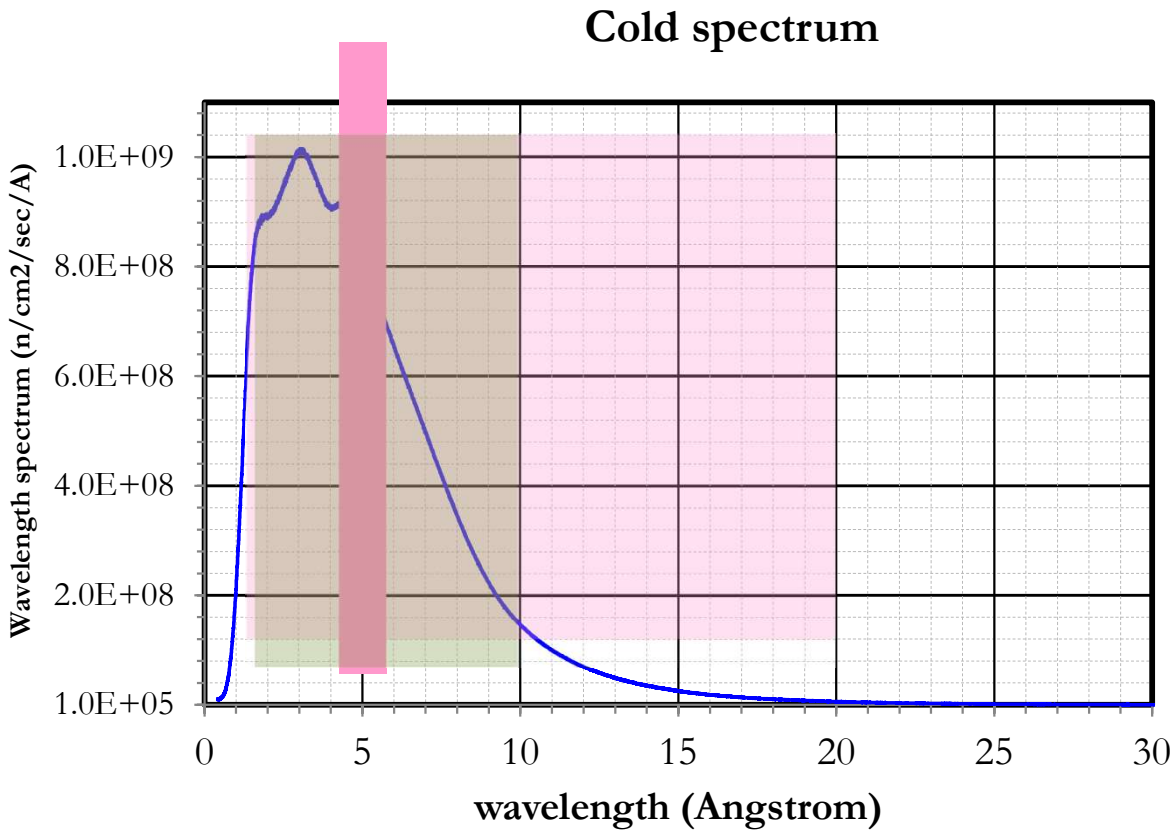
Monochromatic vs polychromatic SANS



March – October 2024:
Cold source replacement
~5% loss at short wavelength, ~5% gain at the long

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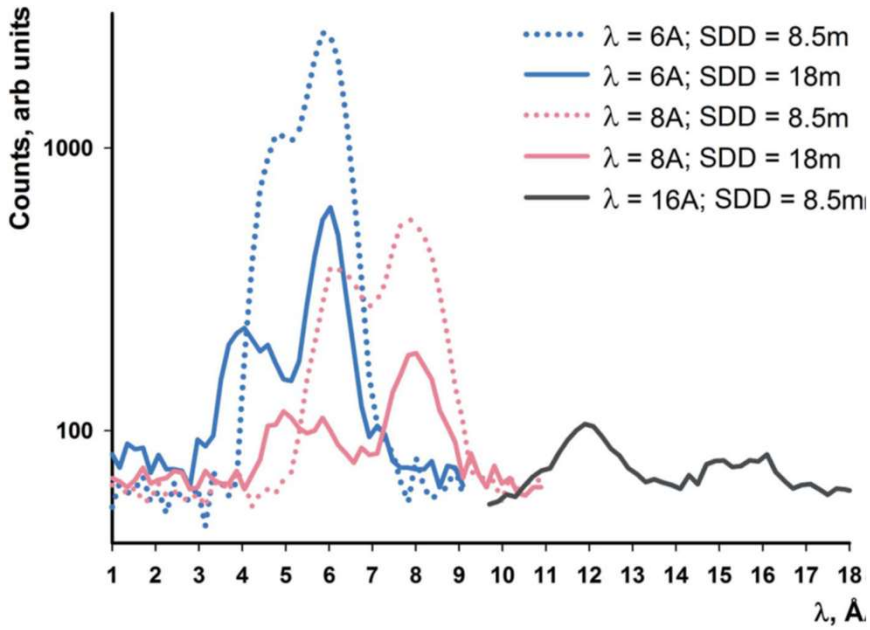
Hydrogen issues: Incoherent / inelastic

Bilby: wavelength contamination is different for different detectors:

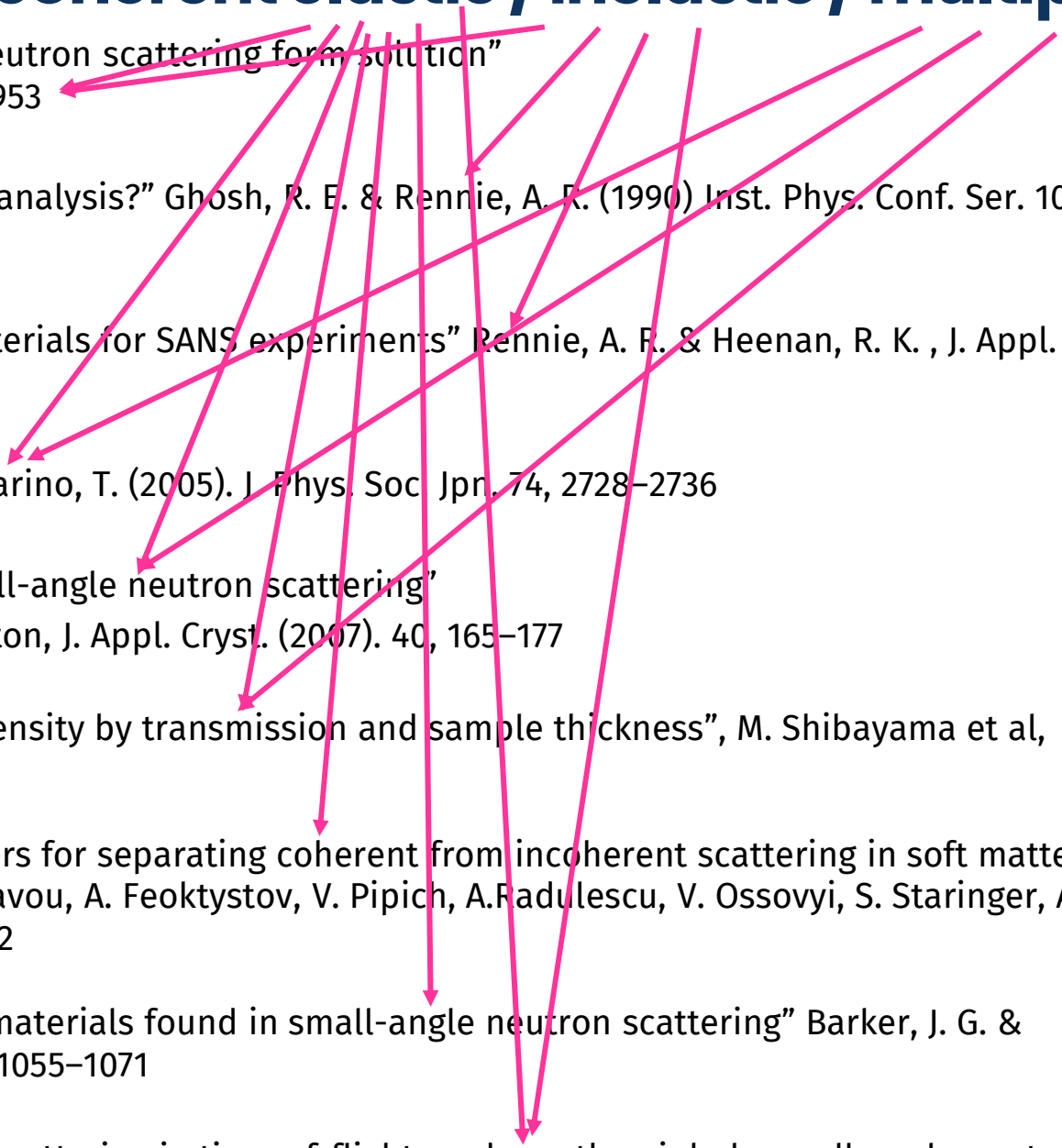


Effective wavelength recorded for **20Å** at L2 of:
2m: **19.97Å**; 5m: **17.4Å**; 10m: **15.5Å**; 18m: **13.15Å**

Effective wavelength recorded for **10Å** at L2 of:
2m: **9.5Å**; 5m: **8.88Å**; 10m: **8Å**; 18m: **7Å**.

Chopper – sample stage distance is ~30m

Hydrogen issues: Incoherent elastic / inelastic / multiple



"The study of biological structures by neutron scattering from solution"
B. Jacrot, Rep. Prog. Phys. (1976) 39, 911-953

"Can we justify conventional SANS data analysis?" Ghosh, R. E. & Rennie, A. R. (1990) Inst. Phys. Conf. Ser. 107, 233–244

"Assessment of detector calibration materials for SANS experiments" Rennie, A. R. & Heenan, R. K. , J. Appl. Cryst. (1999). 32, 1157-1163

Shibayama, M., Nagao, M., Okabe, S. & Karino, T. (2005). J. Phys. Soc. Jpn. 74, 2728–2736

"Improvement of data treatment in small-angle neutron scattering"
A. Brulet, D. Lairez, A. Lapp and J.–P. Cotton, J. Appl. Cryst. (2007). 40, 165–177

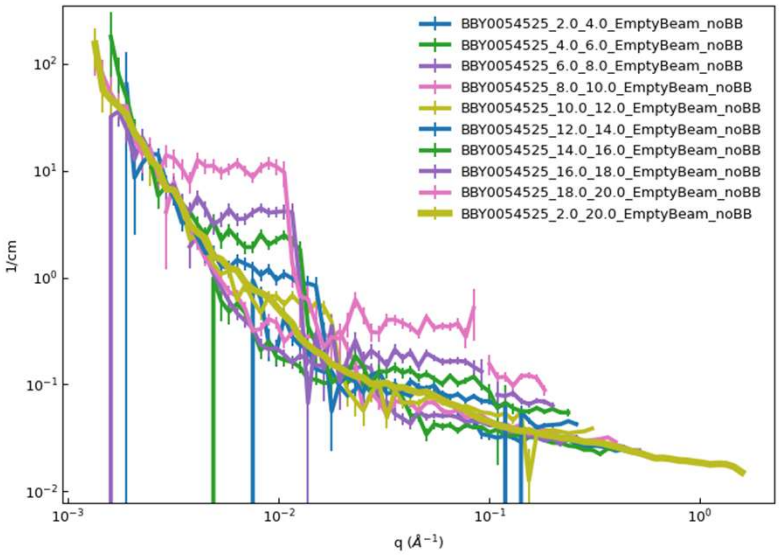
"Evaluation of incoherent scattering intensity by transmission and sample thickness", M. Shibayama et al, J Appl Cryst (2009)

"Polarization analysis with 3He spin filters for separating coherent from incoherent scattering in soft matter studies", E. Babcock, Z. Salhia, M-S. Appavou, A. Feoktystov, V. Pipich, A.Radulescu, V. Ossovyi, S. Staringer, A. Ioffe, Physics Procedia 42 (2013) 154 – 162

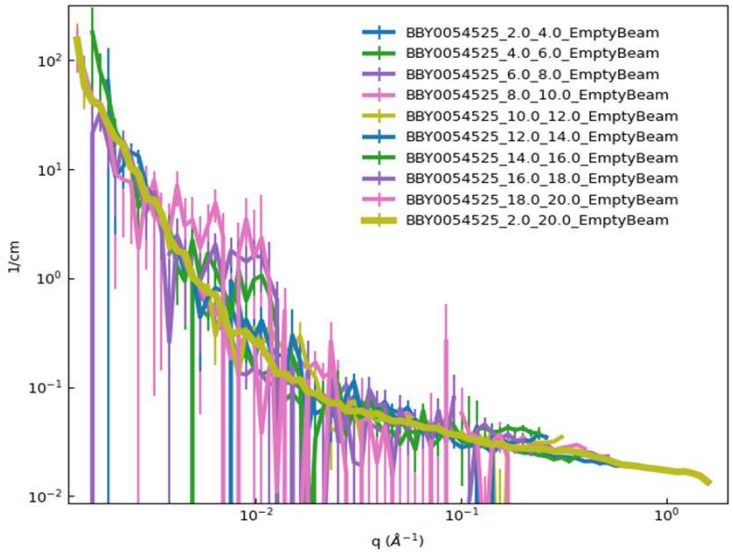
"Survey of background scattering from materials found in small-angle neutron scattering" Barker, J. G. & Mildner, D. F. R. (2015). J. Appl. Cryst. 48, 1055–1071

"Separation of the inelastic and elastic scattering in time-of-flight mode on the pinhole small-angle neutron scattering diffractometer KWS-2", L. Balacescu et al., J. Appl. Cryst. (2021). 54, 1217–1224

Important: backgrounds!!
Even blocked beam – see empty beam scattering:

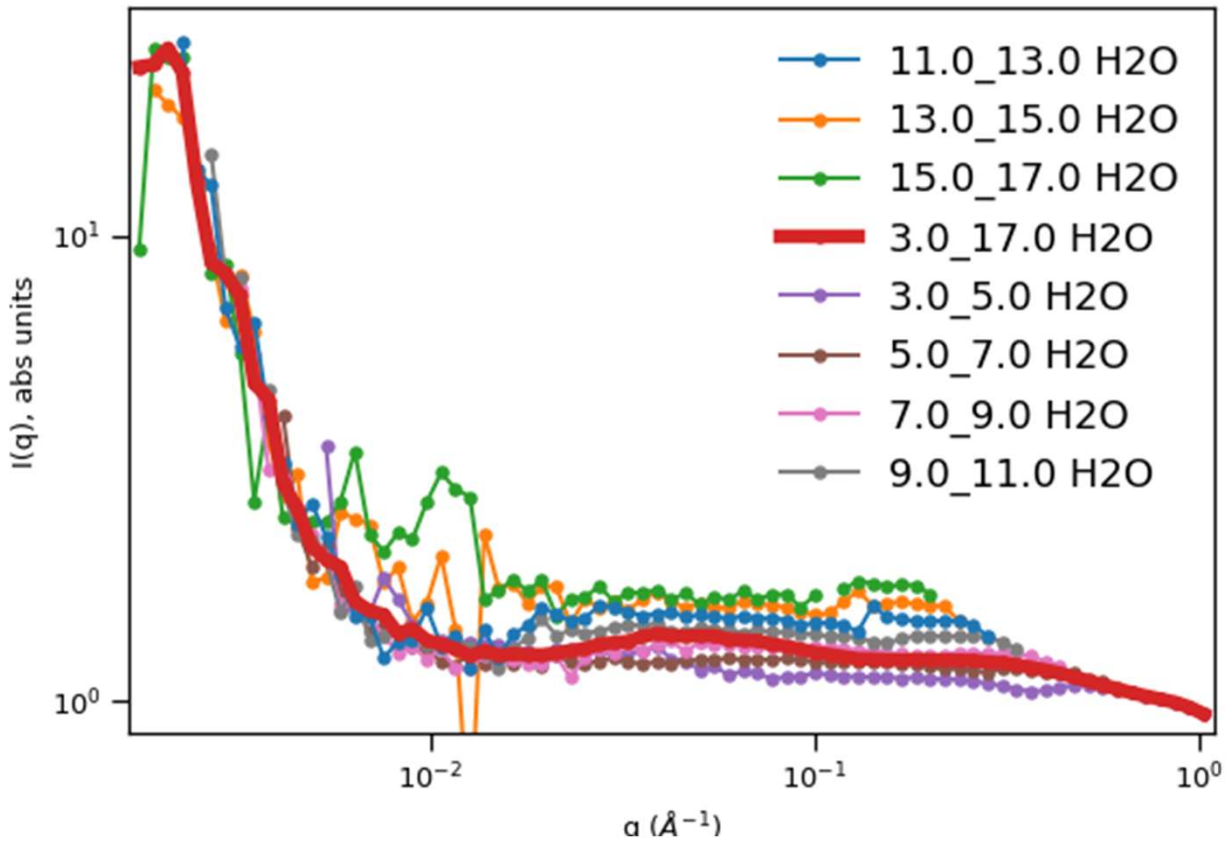


30min



Example: a lot of hydrogen in the solvent

100% H2O



Important: the fake peak on the red curve is NOT ending up published.

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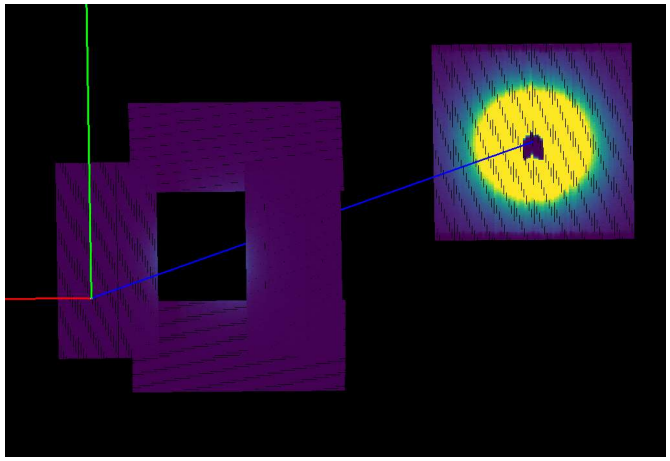
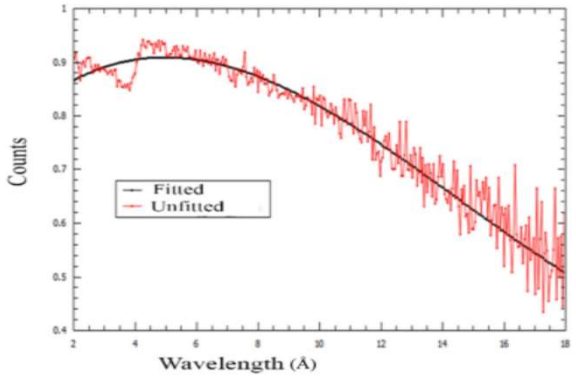
ToF issues: multiple scattering

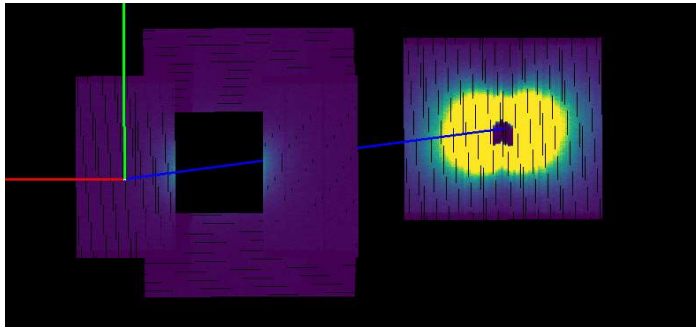
Fe:

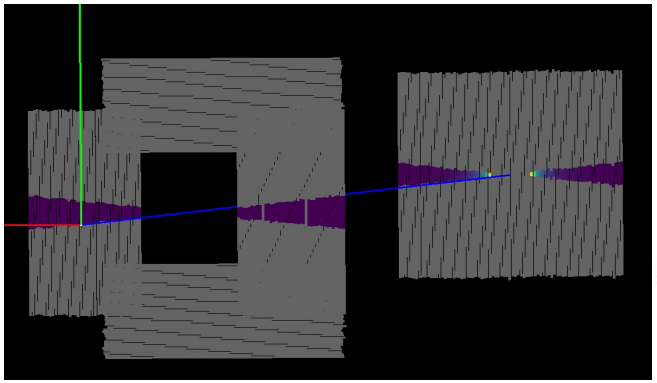


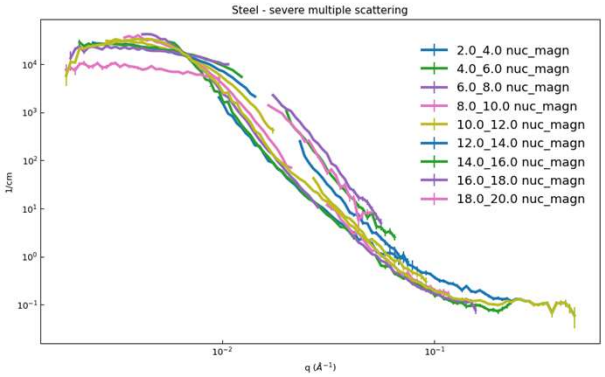
Transmission
Bragg edge



Steel alloy: in the field, multiple scattering – sample is too thick







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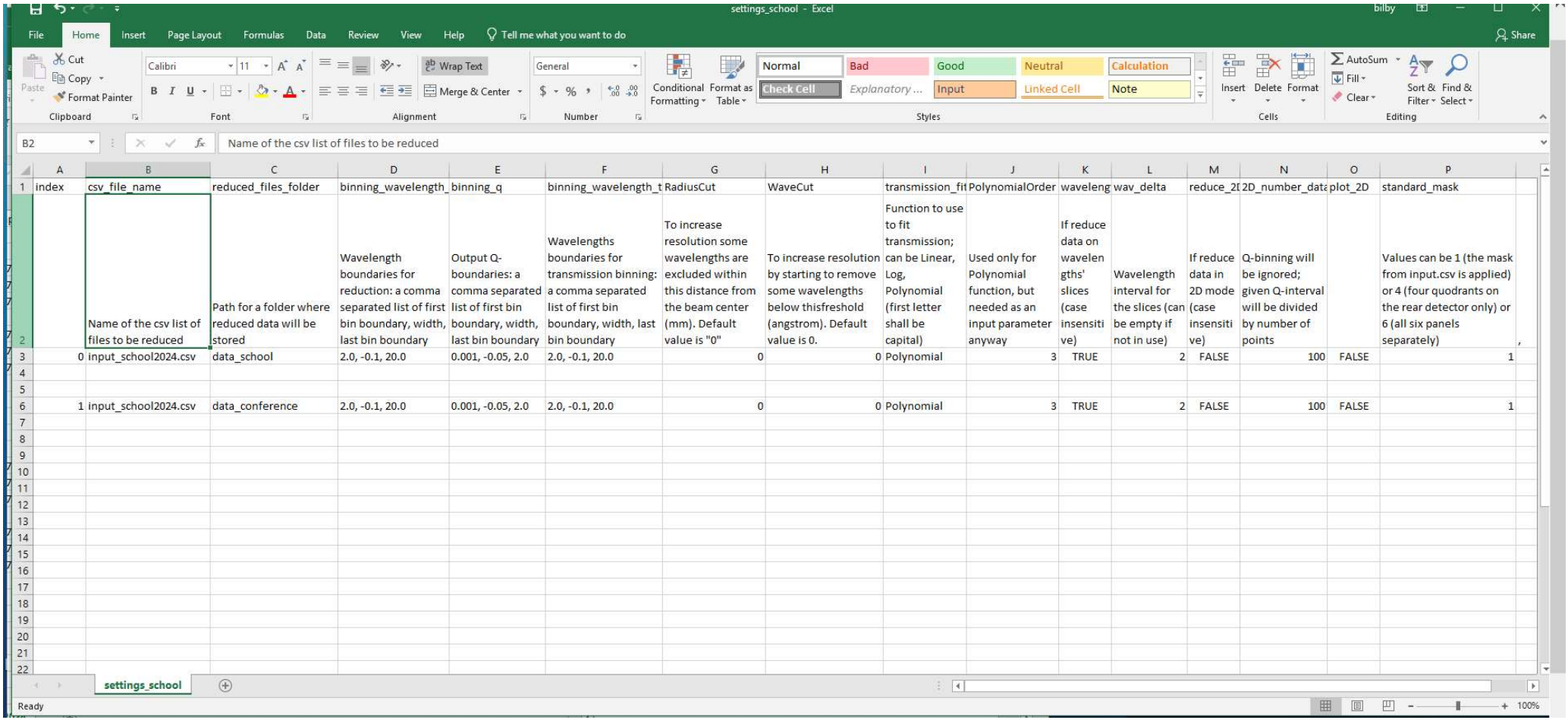
Bilby reduction: settings



settings_school - Excel

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	index	csv_file_name	reduced_files_folder	binning_wavelength_	binning_q	binning_wavelength_t	RadiusCut	WaveCut	transmission_fit	PolynomialOrder	waveleng	wav_delta	reduce_2[	2D_number_data	plot_2D	standard_mask
2		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		Values can be 1 (the mask from input.csv is applied) or 4 (four quodrants on the rear detector only) or 6 (all six panels separately)
3	0	input_school2024.csv	data_school	2.0, -0.1, 20.0	0.001, -0.05, 2.0	2.0, -0.1, 20.0	0	0	Polynomial	3	TRUE	2	FALSE	100	FALSE	1
4																
5																
6	1	input_school2024.csv	data_conference	2.0, -0.1, 20.0	0.001, -0.05, 2.0	2.0, -0.1, 20.0	0	0	Polynomial	3	TRUE	2	FALSE	100	FALSE	1

[Mantid Project — MantidProject landing page documentation]

https://github.com/hortica/Mantid_Bilby

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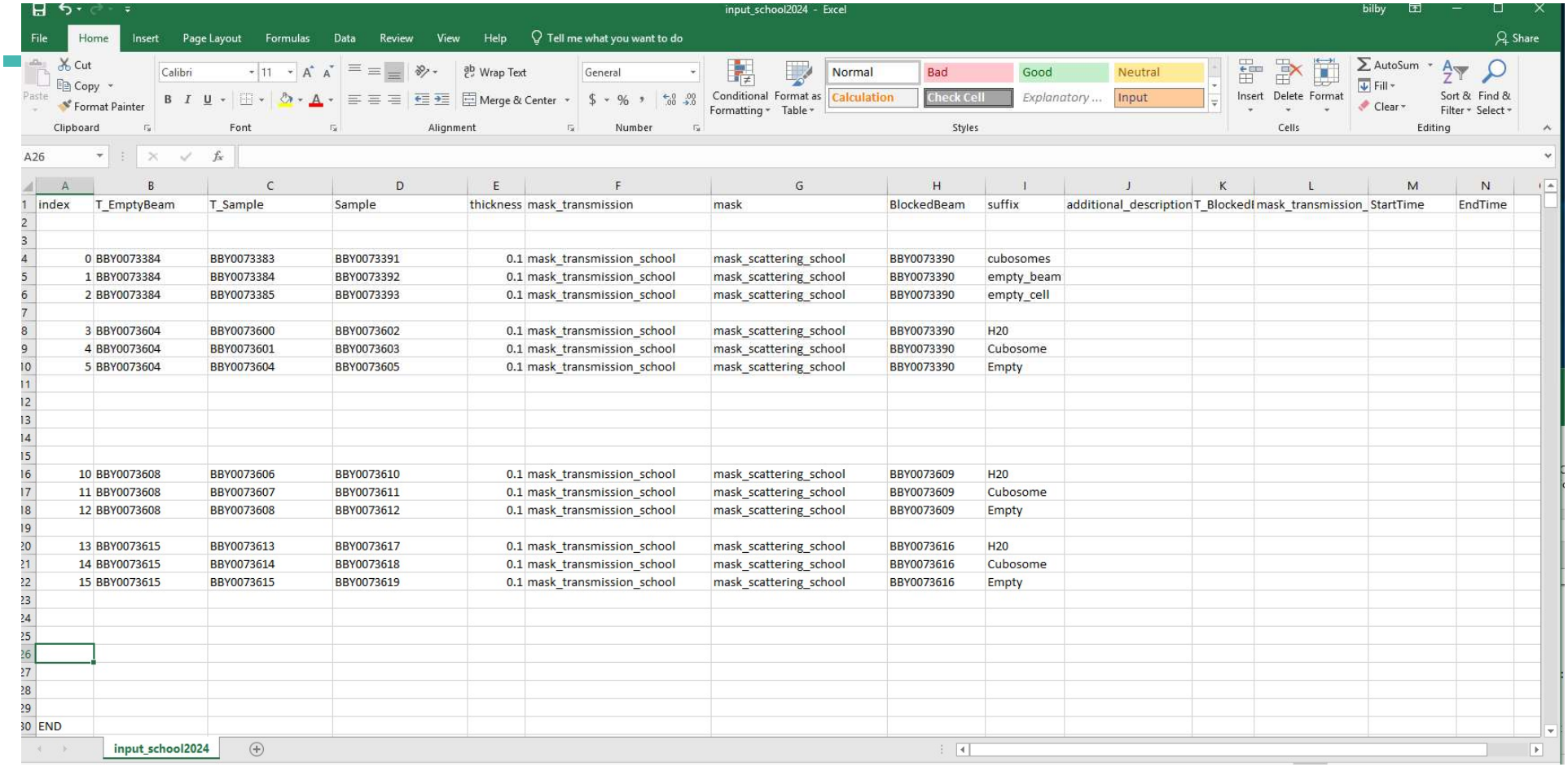
Bilby reduction: list of files



input_school2024 - Excel

index	T_EmptyBeam	T_Sample	Sample	thickness	mask_transmission	mask	BlockedBeam	suffix	additional_description	T_BlockedI	mask_transmission_	StartTime	EndTime
0	BBY0073384	BBY0073383	BBY0073391	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	cubosomes					
1	BBY0073384	BBY0073384	BBY0073392	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	empty_beam					
2	BBY0073384	BBY0073385	BBY0073393	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	empty_cell					
3	BBY0073604	BBY0073600	BBY0073602	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	H20					
4	BBY0073604	BBY0073601	BBY0073603	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	Cubosome					
5	BBY0073604	BBY0073604	BBY0073605	0.1	mask_transmission_school	mask_scattering_school	BBY0073390	Empty					
10	BBY0073608	BBY0073606	BBY0073610	0.1	mask_transmission_school	mask_scattering_school	BBY0073609	H20					
11	BBY0073608	BBY0073607	BBY0073611	0.1	mask_transmission_school	mask_scattering_school	BBY0073609	Cubosome					
12	BBY0073608	BBY0073608	BBY0073612	0.1	mask_transmission_school	mask_scattering_school	BBY0073609	Empty					
13	BBY0073615	BBY0073613	BBY0073617	0.1	mask_transmission_school	mask_scattering_school	BBY0073616	H20					
14	BBY0073615	BBY0073614	BBY0073618	0.1	mask_transmission_school	mask_scattering_school	BBY0073616	Cubosome					
15	BBY0073615	BBY0073615	BBY0073619	0.1	mask_transmission_school	mask_scattering_school	BBY0073616	Empty					
END													

[Mantid Project — MantidProject landing page documentation]

https://github.com/hortica/Mantid_Bilby

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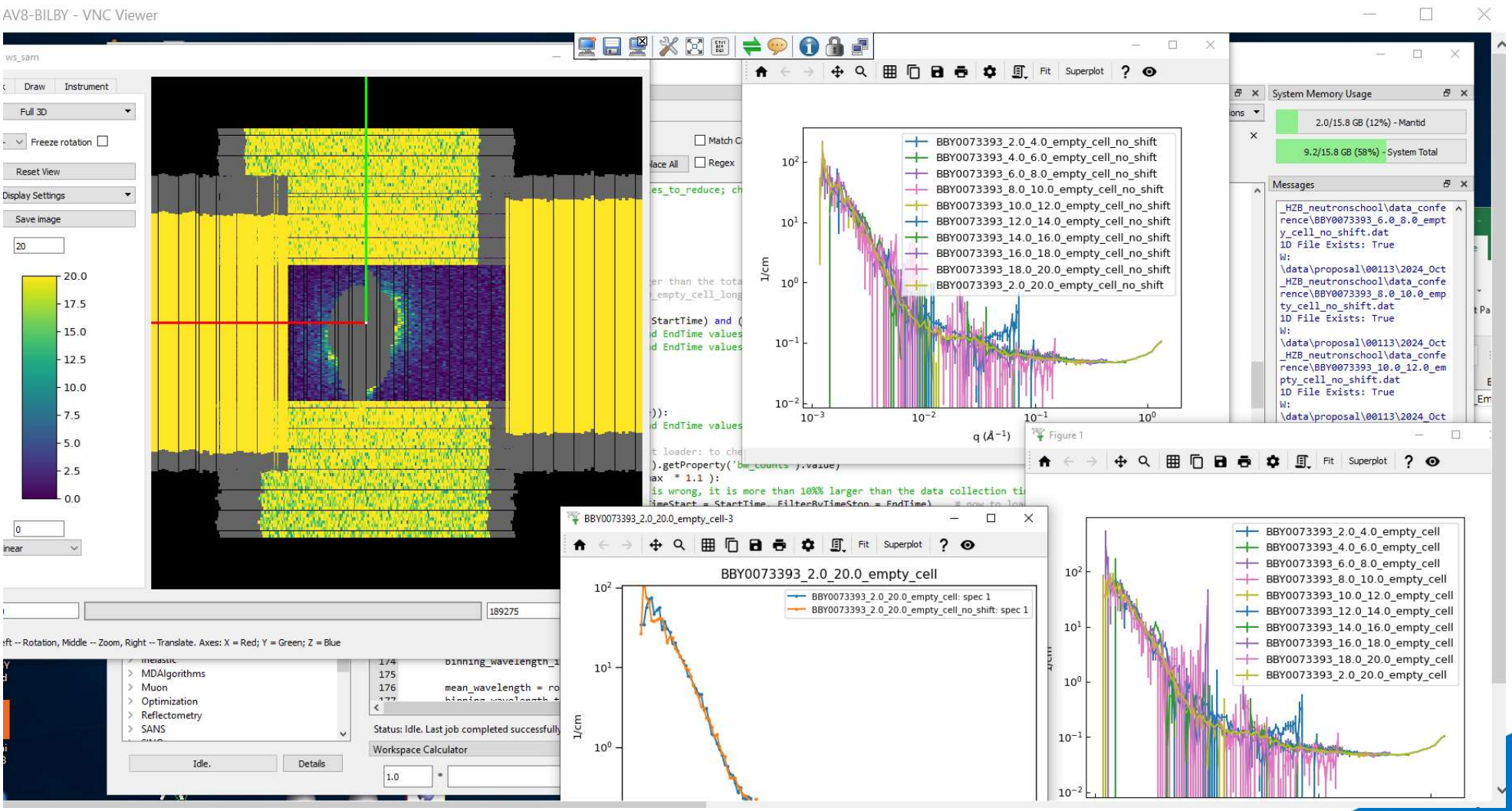
Uncorrected detectors shift: empty cell

Bilby: Liliana de Campo convinced me to try the reduction on unshifted detectors



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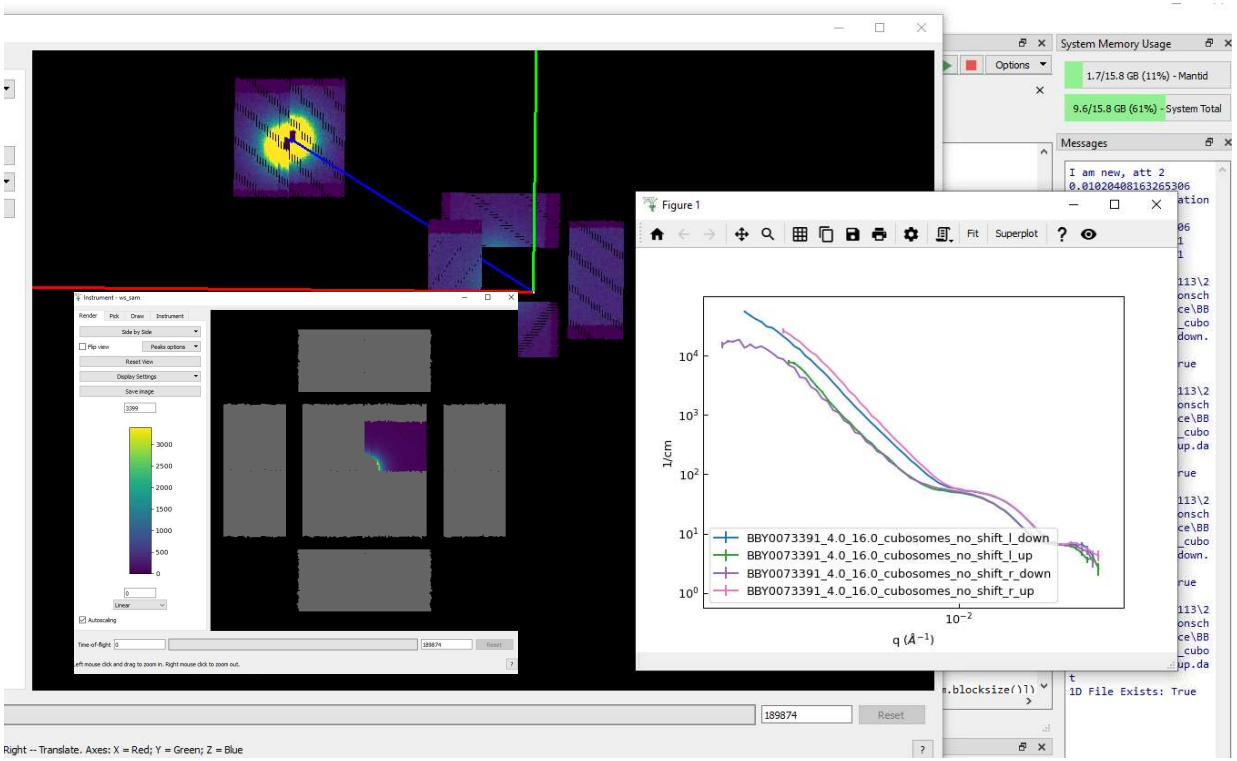
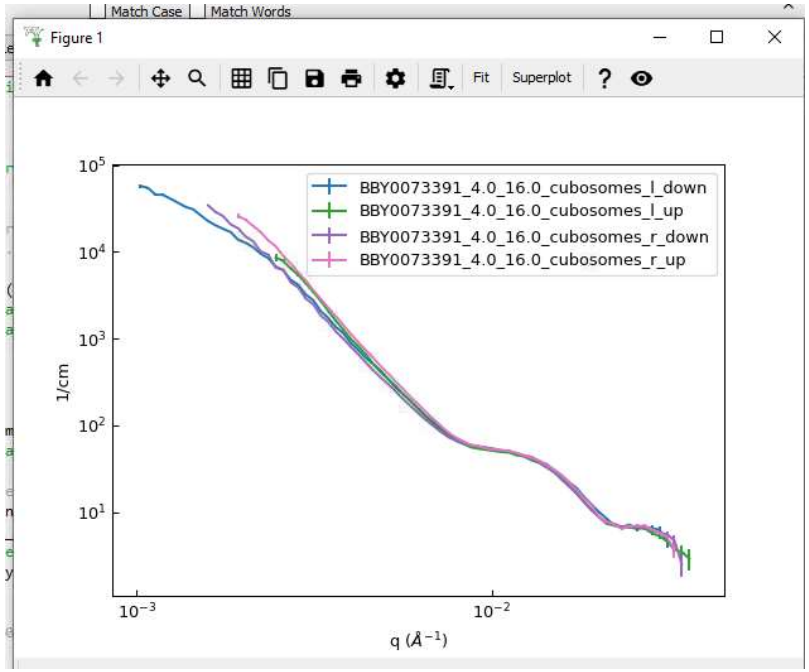
Uncorrected & corrected detectors shift: cubosomes

Bilby: Liliana de Campo' sample

Here: importance of checking data on each quadrant – when averaged, all features gone (see next).



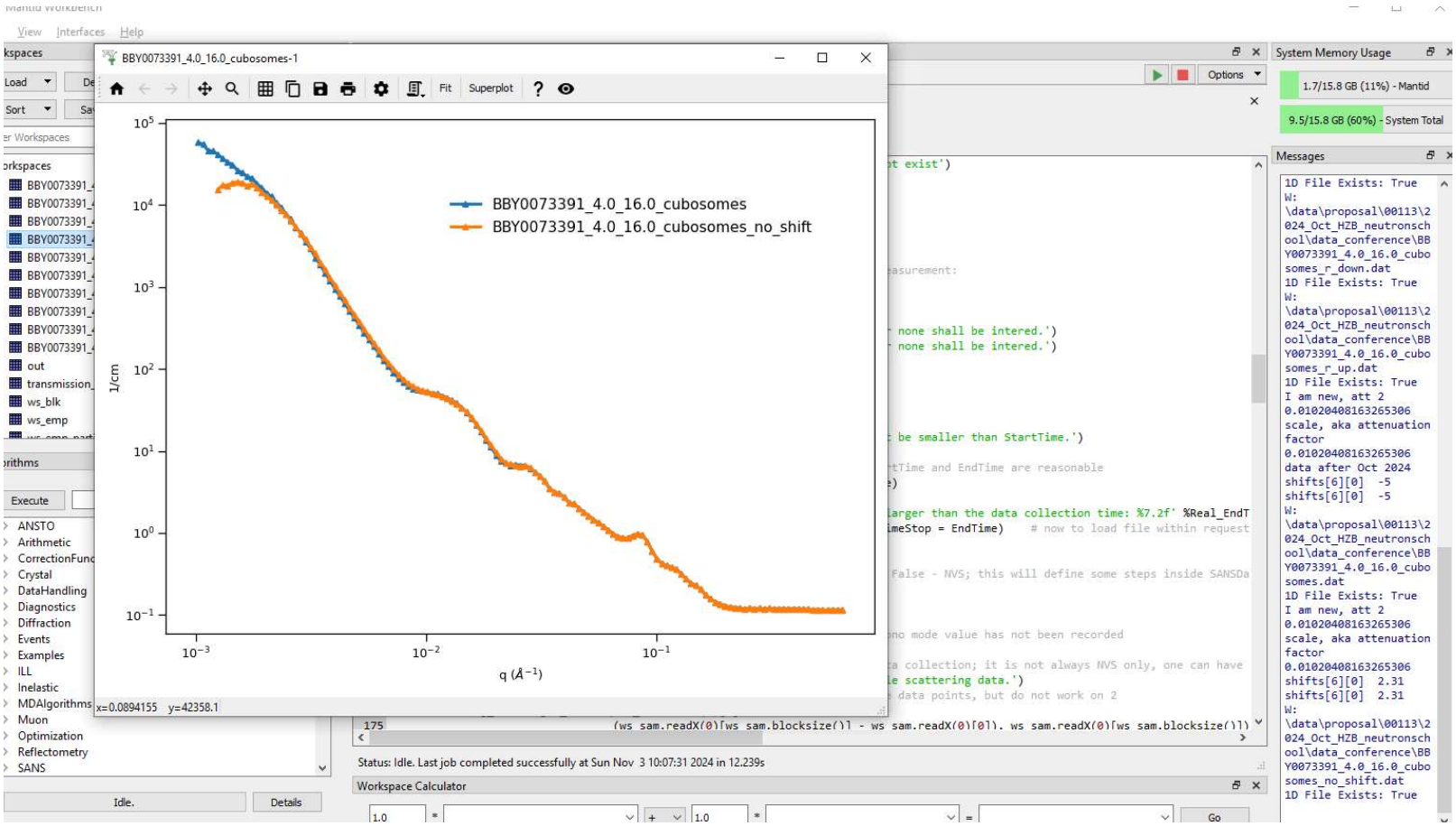


Mantid Project — MantidProject landing page documentation

https://github.com/hortica/Mantid_Bilby

Uncorrected & corrected detectors shift: cubosomes

Here: importance of checking data on each quadrant – when averaged, all features gone. Averaged data look nearly identical (speaking only low Q here).



Quality of the data

Bilby reduction: a lot of options – history can be recovered.

Strong scattering: forgiving for the shifts in detectors, unless looked at quadrants

-> *extra check for the anysometry!*

Incoherent: a lot of extra peaks published – not real.

Users: Jupiter notebooks & the rest: how many things are going to be missed???

Me & P. Butler here

- **Current open questions:**
  - SAXS high Q background subtraction? Any more on SAXS?
  - TOF SANS background subtraction issues from strongly hydrogenated samples (multiple, incoherent, inelastic scattering).
  - Resolution for TOF SANS (WG already working on this) & SAXS?
- **As mentioned for Bilby – above: transparency of the code (more work for local contacts… but – peace of mind)**
  - Autoscaling different configurations: background scaling, different resolution.
  - Various background subtraction can cause artificial feature to appear.
  - The wrong backgrounds / sensitivity was not applied (though sensitivity is not much of a drama for ToF).
- **How can these be captured?**
  - Publication guidelines? Like J. Trewhella (+ Hamburg group) for bioSANS/SAXS data?
- **Future: Pipelining and reduction on the fly (autoreduction)**
  - BUT - given above how to make sure it is done correctly for the current experiment? Is this an area where for AI/ML?
  - How do we maintain transparency on reduction in an age of automation? Do database repositories have a role here?
  - What about the growing push from publishers to publish the reduction and analysis.

  (Hard to publish intermediate results, not always available as outputs.)