

Mantid Update from the MLZ

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Outline

- Heinz-Maier-Leibnitz Zentrum (MLZ) and FRM-II operation status
- Development of new and maintenance of existing tools at MLZ:
 - GUI for TOFTOF
 - Loader for SANS-1 and data reduction in Mantid
 - New GUI for DNS: support of data reduction for 3 operational modes of the instrument and future improvements
- Summary

Heinz Maier-Leibnitz Zentrum (MLZ)

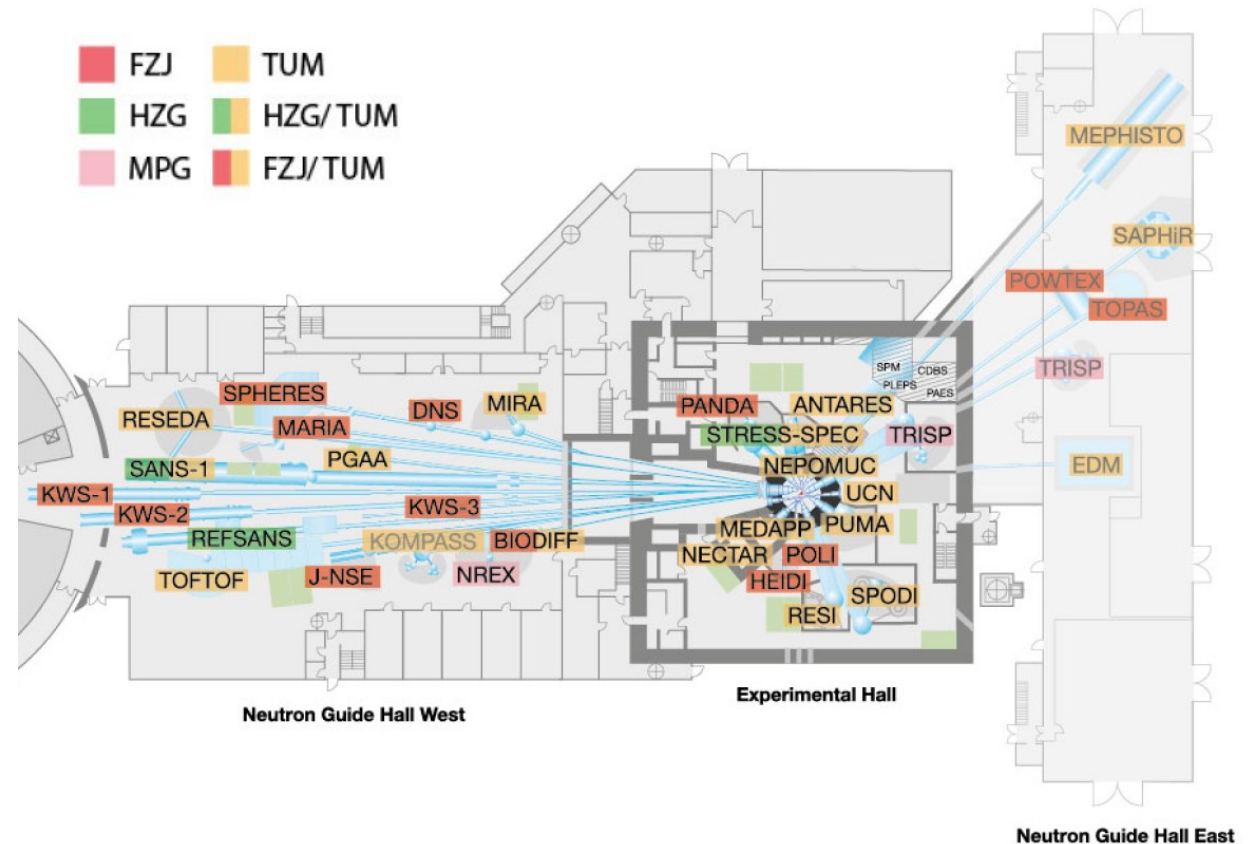
- FRM-II – research reactor and source of neutrons. Operated by TUM.
- Heinz Maier-Leibnitz Zentrum (MLZ) located in Garching near Munich.
- MLZ is cooperation between:
 - Technische Universität München (TUM)
 - Forschungszentrum Jülich (FZJ/JCNS)
 - Helmholtz-Zentrum Hereon
 - Max-Planck-Society



<https://mlz-garching.de/ueber-mlz>

MLZ Instrument Suite

- ~30 scientific instruments, 5 in construction
- No operation since 2020/2021:
 - Failure of cold source → new cold source needs to be manufactured. Projected delivery: mid 2027.
 - Slight leak in the central channel → new central channel needs to be manufactured. Projected delivery: fall 2026. Reactor operation with thermal neutrons is expected.
- East Guide Hall commencement is expected right after the reactor restart.



Maintenance of interface for TOFTOF

- TOFTOF - direct geometry disc-chopper time-of-flight spectrometer.
- Suitable for inelastic and quasi-elastic neutron scattering.
 - dynamics in disordered materials
 - low-energy magnetic excitations in multiferroic compounds & molecular magnets
- Uses DGS Reduction interface for data reduction. Currently in maintenance.
- DEVA-QENS workshop, 02.12.2025. Demo on QENS data reduction and analysis using Mantid.

<https://indico.frm2.tum.de/event/458/>

TOFTOF Reduction: /mantid_data/toftof/data/TOFTOF_reduction.xml

File Tools

TOFTOF Reduction

Data search directory: /mantid_data/toftof/data [Browse]

Workspace prefix: ws

Inputs

Vanadium runs: 44512:44514

Van. comment: Van_res EC factor: 1.000 T (K):

Empty can runs: 44515:44517 EC factor: 0.900 T (K):

Mask detectors:

Binning

	on start	step	end
Energy	☒ -6.000	0.0100	1.800
Q	☒ 0.400	0.100	2.000

Options

☒ Subtract empty can from vanadium

Normalise: ☐ none ☒ to monitor ☐ to time

Correct TOF: ☐ none ☒ vanadium ☐ sample

☐ Replace special values in $S(Q, \omega)$ with 0

☐ Create diffractograms

☐ Keep intermediate steps

Data

Data runs	Comment	T (K)
44527:44529	H2O_21C	
44530:44531	H2O_34C	

☐ Save reduced data

Directory: [Browse]

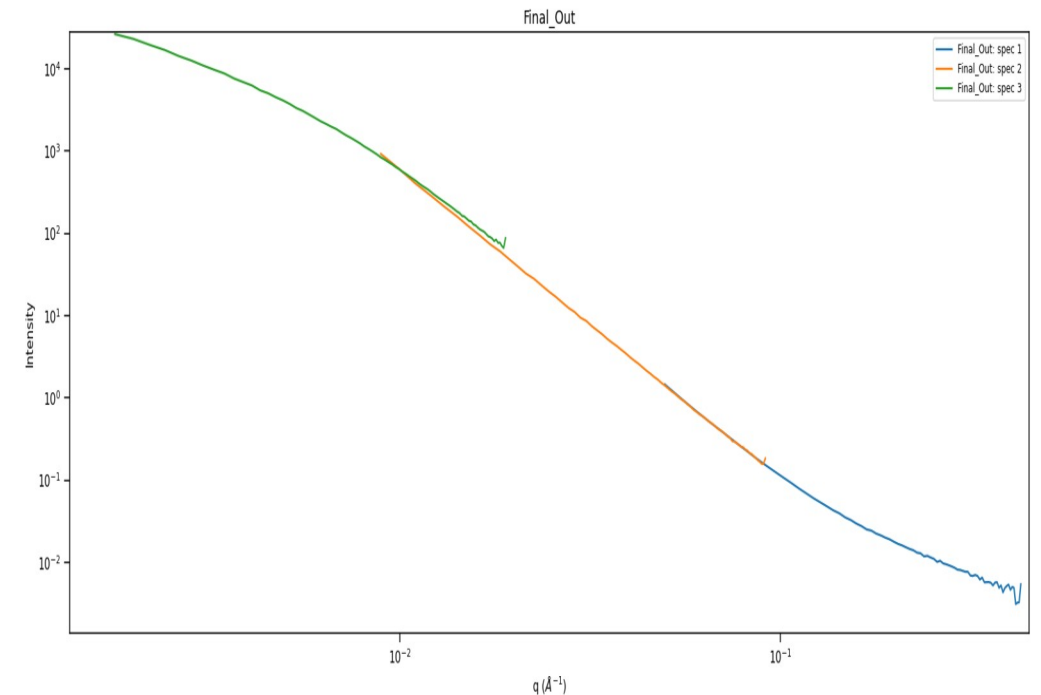
$S(Q, \omega)$: ☐ NeXus ☐ Ascii

$S(2\theta, \omega)$: ☐ NeXus ☐ Ascii ☐ NXSPE

[Reduce] [Save] [Export]

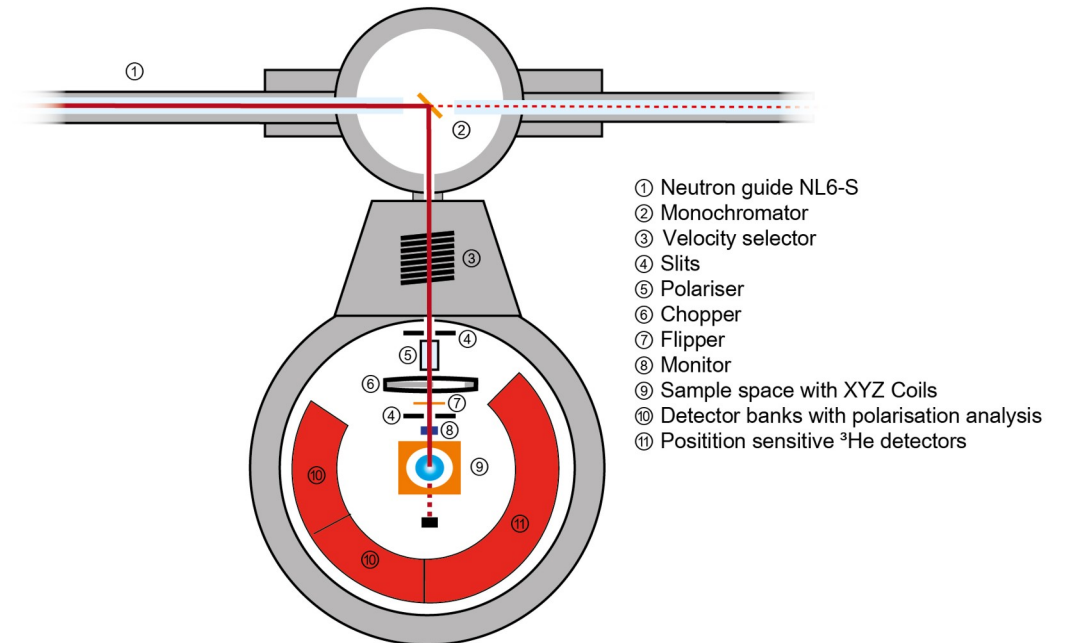
Loader and data reduction script for SANS-1

- SANS-1: small angle neutron scattering instrument. Operated by TUM & Hereon.
- “LoadSANS1MLZ” – loads SANS-1 data into a ws. Developed by A. Demydenko. Provides an alternative to using no longer BerSANS GUI.
- SANS-1 data reduction workflow can be reproduced using “SANSILLReduction” algorithm. Data reduction script was developed.



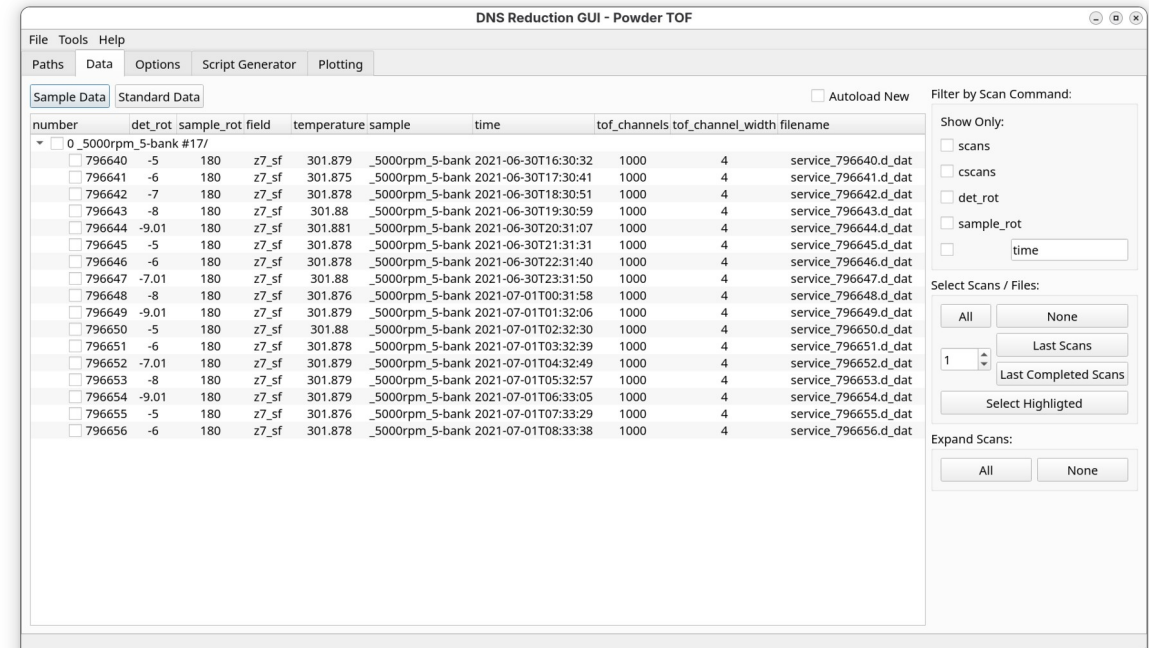
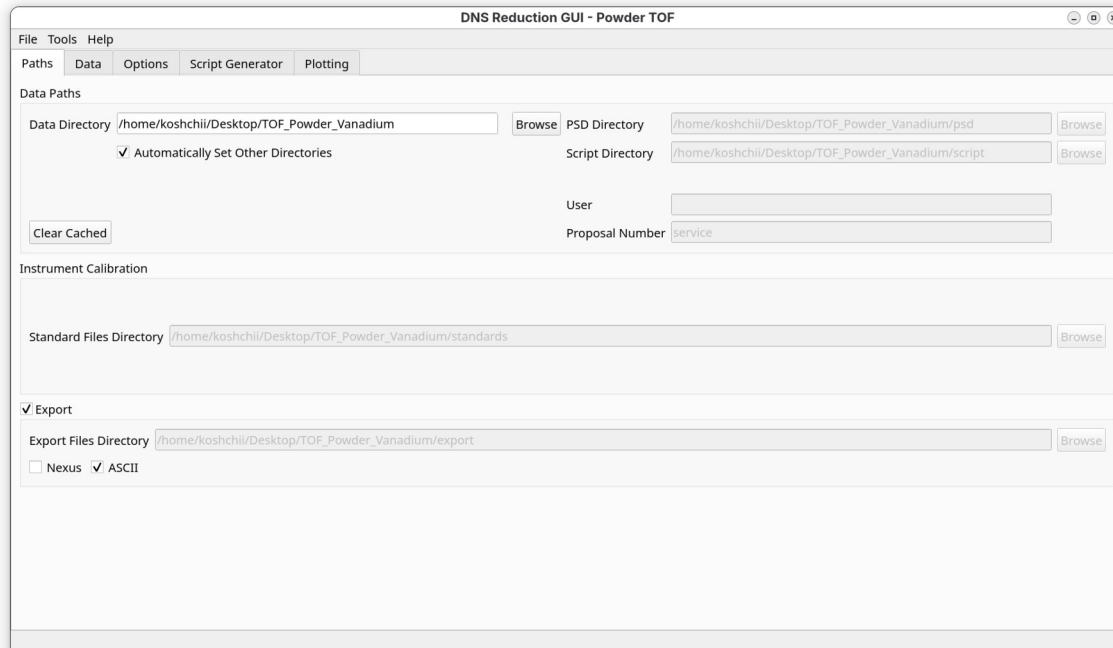
DNS Reduction Interface

- DNS: polarised neutron scattering instrument with time-of-flight inelastic scattering option. Operated by FZJ, similar to D7@ILL.
- Polarisation analysis (PA) bank: 24 detectors, angular resolution 5° . Operation with PSD bank (128 detectors, 960 pixels each) also possible.
- Development of “DNS Reduction” GUI started by T. Müller in collaboration with M. Ganeva, picked up by O. Koshchii. Replaces no longer supported DNSPlot interface.
- At the moment, supports data reductions for 3 different operational modes of DNS.



https://docs.mantidproject.org/nightly/interfaces/direct/dns_reduction/DNS%20Reduction.html

DNS Reduction: Common Features



- 3 operational modes share common “Path” & “Data” & “Script Generator” widgets.
- Dedicated “Options” & “Plotting” widgets for each mode of operation.
- Each scan (rotation) is saved as a separate file and loaded into a separate workspace. As a result of data reduction, a merged workspace is generated.

DNS Powder TOF

- Powder TOF: deployed in Fall 2022 (release v6.5).
- Event mode data, up to 1024 time channels.
Operation without polarisation analysis.
- Study low-energy magnetic excitations.
- Data reduction:
 - Counts normalisation
 - Detector efficiency
 - Background correction that can take into account self-shielding factor
 - Elastic peak position correction, which uses vanadium peak fit to shift elastic peak position to 0 meV
 - Transformation to (Q , ω)

The screenshot shows the 'DNS Reduction GUI - Powder TOF' window. It features a menu bar (File, Tools, Help) and a tabbed interface with 'Paths', 'Data', 'Options', 'Script Generator', and 'Plotting'. The 'Options' tab is active, displaying various configuration settings:

- Wavelength (Angstrom):** A dropdown menu showing '4.74' and a checkbox for 'Get from Data'.
- Normalisation:** Radio buttons for 'No' and 'Monitor'.
- Corrections:** A checked section containing:
 - Detector Efficiency Correction:** A checked checkbox with a 'Vanadium Temperature' input field set to '295.00'.
 - Subtract Instrument Background from Vanadium:** A checked checkbox with a 'Factor' input field set to '1.00'.
 - Correct Elastic Peak Position to 0 meV:** A checked checkbox.
 - Mask Bad Detectors (Vanadium Counts < 0):** An unchecked checkbox.
 - Subtract Instrument Background from Sample:** A checked checkbox with a 'Factor' input field set to '1.00'.
- TOF Options:** An 'Elastic Peak Channel' input field set to '0' and a checked checkbox for 'Delete Raw Workspaces'.
- Binning:** Input fields for 'q minimum' (0.116), 'q maximum' (2.837), 'q step size' (0.025), 'dE minimum' (-3.141), 'dE maximum' (3.141), and 'dE step size' (0.073). A 'Suggest From Data' button is located below these fields.

DNS Powder TOF

```

DNS Reduction GUI - Powder TOF
File Tools Help
Paths Data Options Script Generator Plotting

Generate and Run Script Filename: script_5000rpm_5-bank_from_796640_to_796656.py [x] Automatic Script Filename [Copy Script to Clipboard]

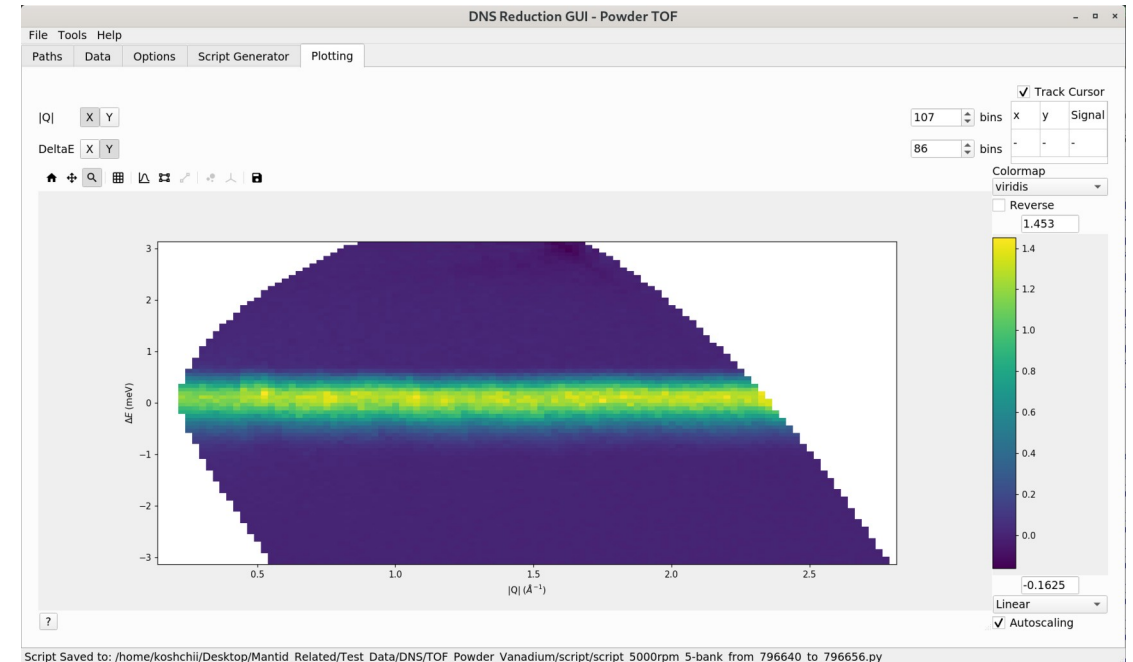
sample_data = {
  '_5000rpm_5-bank': {'path': '/home/koshchii/Desktop/TOF_Powder_Vanadium/service_*****.d_dat',
    -9.00: [796644, 796649, 796654],
    -8.00: [796643, 796648, 796653],
    -7.00: [796642, 796647, 796652],
    -6.00: [796641, 796646, 796651, 796656],
    -5.00: [796640, 796645, 796650, 796655]},
}
standard_data = {
  '_kns0_15000rpm_RT_1-bank_empty_can_data': {'path': '/home/koshchii/Desktop/TOF_Powder_Vanadium/standards/pi3656_*****.d_dat',
    -5.00: [557295]},
  '_vana': {'path': '/home/koshchii/Desktop/TOF_Powder_Vanadium/standards/service_*****.d_dat',
    -5.00: [796640]},
}
params = {'e_channel': 0,
  'wavelength': 4.74,
  'delete_raw': True,
  'vana_temperature': 295.0,
  'ecvanaFactor': 1.0,
  'ecsampleFactor': 1.0,}
bins = {'q_min': 0.110,
  'q_max': 2.037,
  'q_step': 0.025,
  'dE_min': -3.141,
  'dE_max': 3.141,
  'dE_step': 0.073}

load_data(sample_data['_5000rpm_5-bank'], "raw_data1", params)
load_data(standard_data['_kns0_15000rpm_RT_1-bank_empty_can_data'], "raw_ec", params)
load_data(standard_data['_vana'], "raw_vanadium", params)

# normalize
data1 = MonitorEfficiencyCorUser("raw_data1")
ec = MonitorEfficiencyCorUser("raw_ec")
# only one empty can bank
ec = ec[0]
# subtract empty can
data1 = data1 - ec * params['ecsampleFactor']

vanadium = MonitorEfficiencyCorUser("raw_vanadium")
vanadium = vanadium - ec
# only one vanadium bank position
vanadium = vanadium[0]

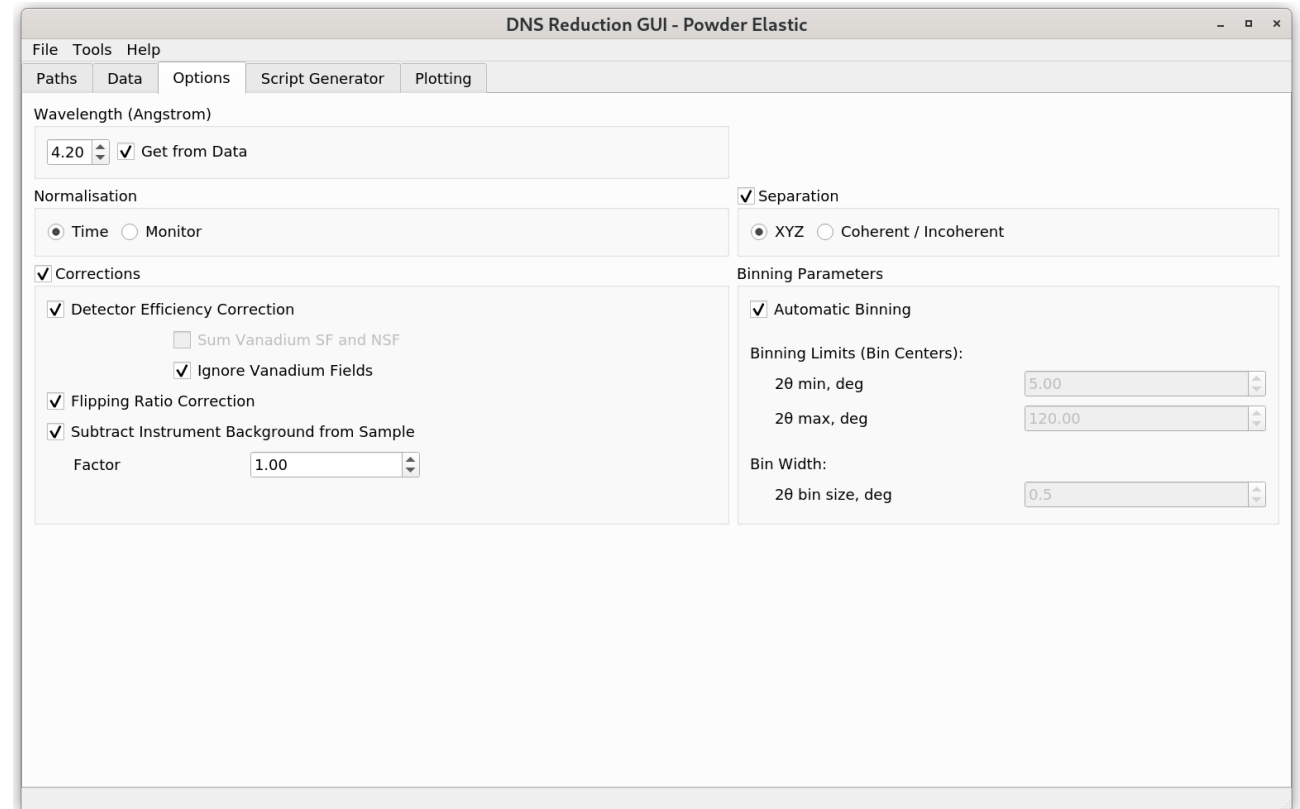
```



- User-friendly python script is generated and executed to create the output.
- The script can be saved to reproduce the workflow later on.
- Sliceviewer is embedded for visualization purposes.

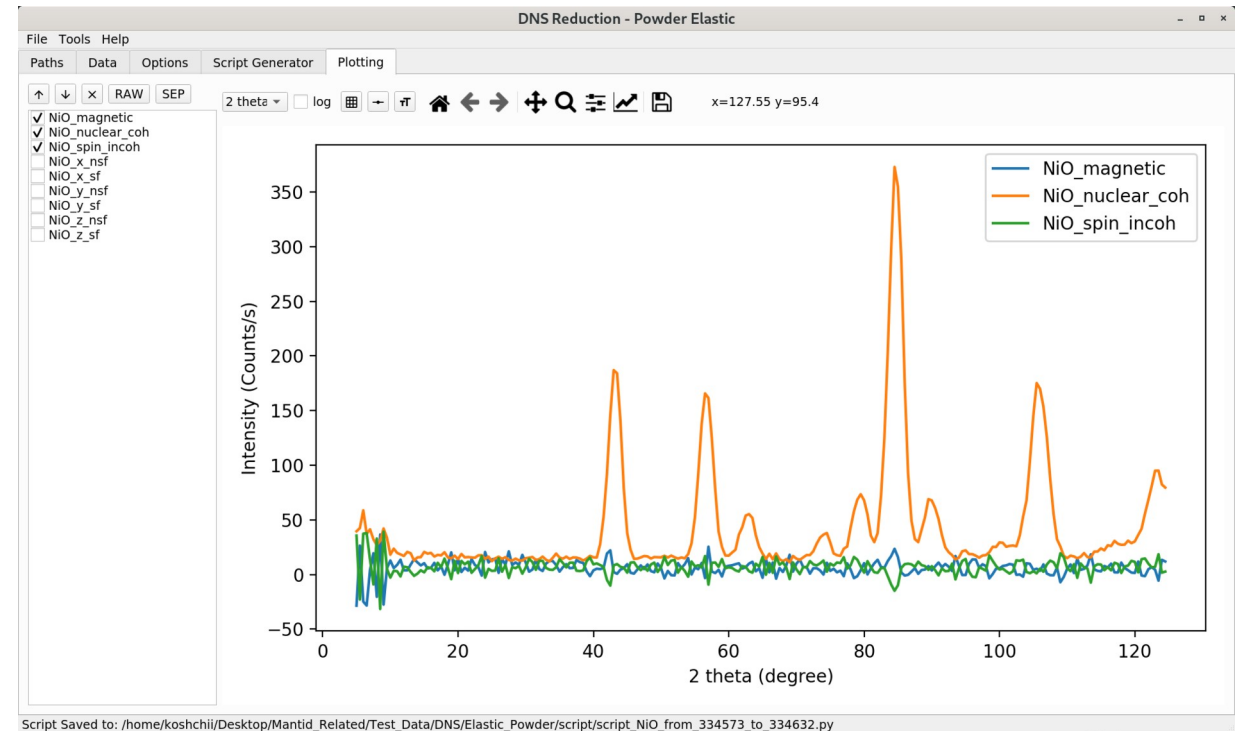
DNS Powder Elastic

- Powder Elastic: deployed in Fall 2023 (release v6.8).
- Typically used in combination with PA.
- xyz-polarisation analysis method is used to separate incoherent/coherent/magnetic scattering contributions.
- Applications:
 - Magnetic diffuse scattering
 - Polarised powder diffraction
 - Coherent/incoherent scattering separation in soft condensed matter



DNS Powder Elastic

- Resulting data are merged into “Workspace2D”.
- Dedicated plotting tool for investigation and visualisation of separated components.
- Features to be implemented:
 - Simultaneous processing of scans measured at different temperatures and possibility to compare in “Plotting” tab.
 - Multiple scattering correction using data-driven evaluation approach.
 - Preliminary data evaluation using Gaussian processes regression.



DNS Single Crystal Elastic

- Single Crystal Elastic: deployment aimed in winter 2025 (release v6.15), 2 PRs to go.
- Polarised single-crystal neutron diffraction.
- Toolbox for data reduction corrections options.
- Sample lattice parameters or d-spacings values selection options.
- Orientation box for specifying horizontal scattering plane.

DNS Reduction GUI - Single Crystal Elastic

File Tools Plot View Plot Options Help

Paths Data Options Script Generator Plotting

Wavelength (Angstrom)

4.20 ☒ Get from Data

Normalisation

☒ Time ☐ Monitor

☒ Corrections

☒ Detector Efficiency Correction

☐ Sum Vanadium SF and NSF

☒ Ignore Vanadium Fields

☒ Flipping Ratio Correction

☒ Subtract Instrument Background from Sample

Factor 1.00

Orientation

n_x , [hkl] 1,1,0

n_y , [hkl] 1,-1,0

ω offset, deg 0.00

☐ Use d-spacings Instead of Lattice Parameters

d_x , Å 3.67

d_y , Å 6.36

Lattice Parameters

a, Å 7.343

b, Å 7.343

c, Å 4.114

α , deg 90.000

β , deg 90.000

γ , deg 120.000

Binning Parameters

☒ Automatic Binning

Binning Limits (Bin Centers) :

2θ min, deg 6.01 ω min, deg 135.01

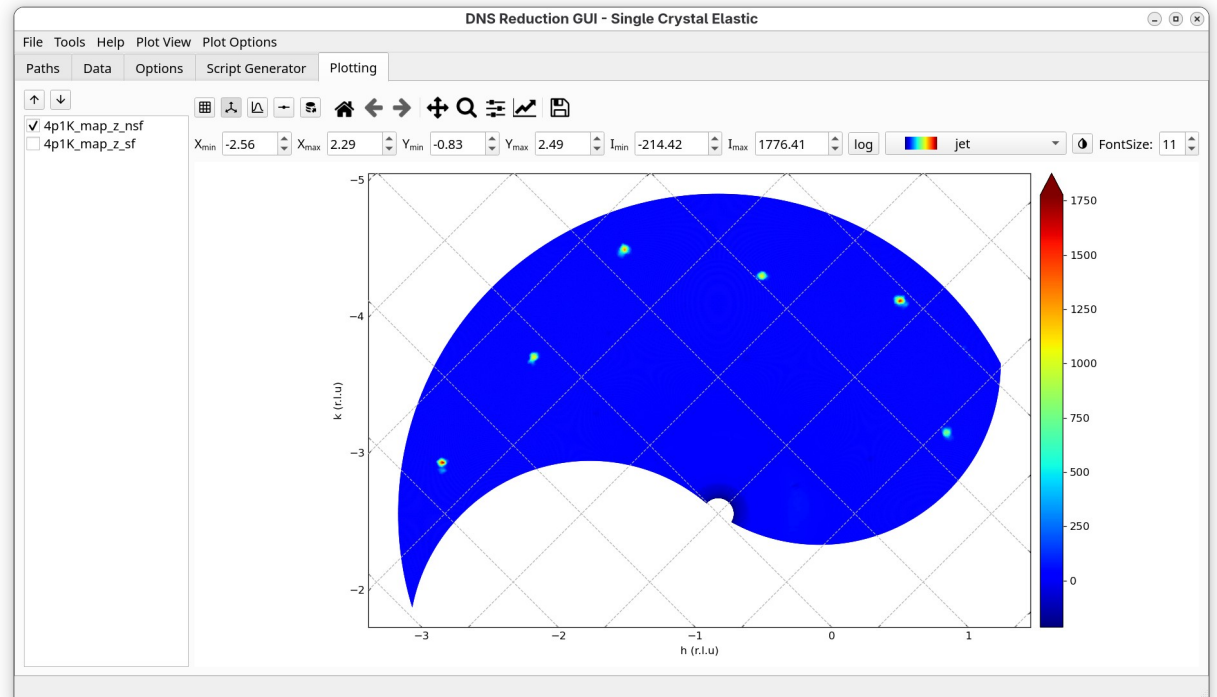
2θ max, deg 121.01 ω max, deg 304.01

Bin Width:

2θ bin size, deg 0.50 ω bin size, deg 1.00

DNS Single Crystal Elastic

- Multiple sample and detector bank rotation scans for each polarisation channel are merged and processed together.
- “LoadDNSSCD” loads all measurement files into a single “MDEventWorkspace”.
- Dedicated “Plot View” and “Plot Options” tabs:
 - “Scatterplot”, “Triangulation”, “Quadmesh” plotting type options
 - Axes transformation options: $(2\theta, \omega)$, (Q_x, Q_y) and (n_x, n_y)
 - Omega offset and d-spacing modification tool
 - Interpolation properties selector



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- Zamaan Raza
- ILL, ORNL and STFC Mantid Teams

Summary

- TOFTOF – in operation, under maintenance
- SANS-1 – loader and data reduction script have been developed
- DNS Reduction:
 - “Powder TOF” and “Powder Diffraction” are in operation, under maintenance, several additional features are in development
 - “Elastic Single Crystal”, development complete, full deployment envisioned by the end of this year
 - “Simulation” mode is in development