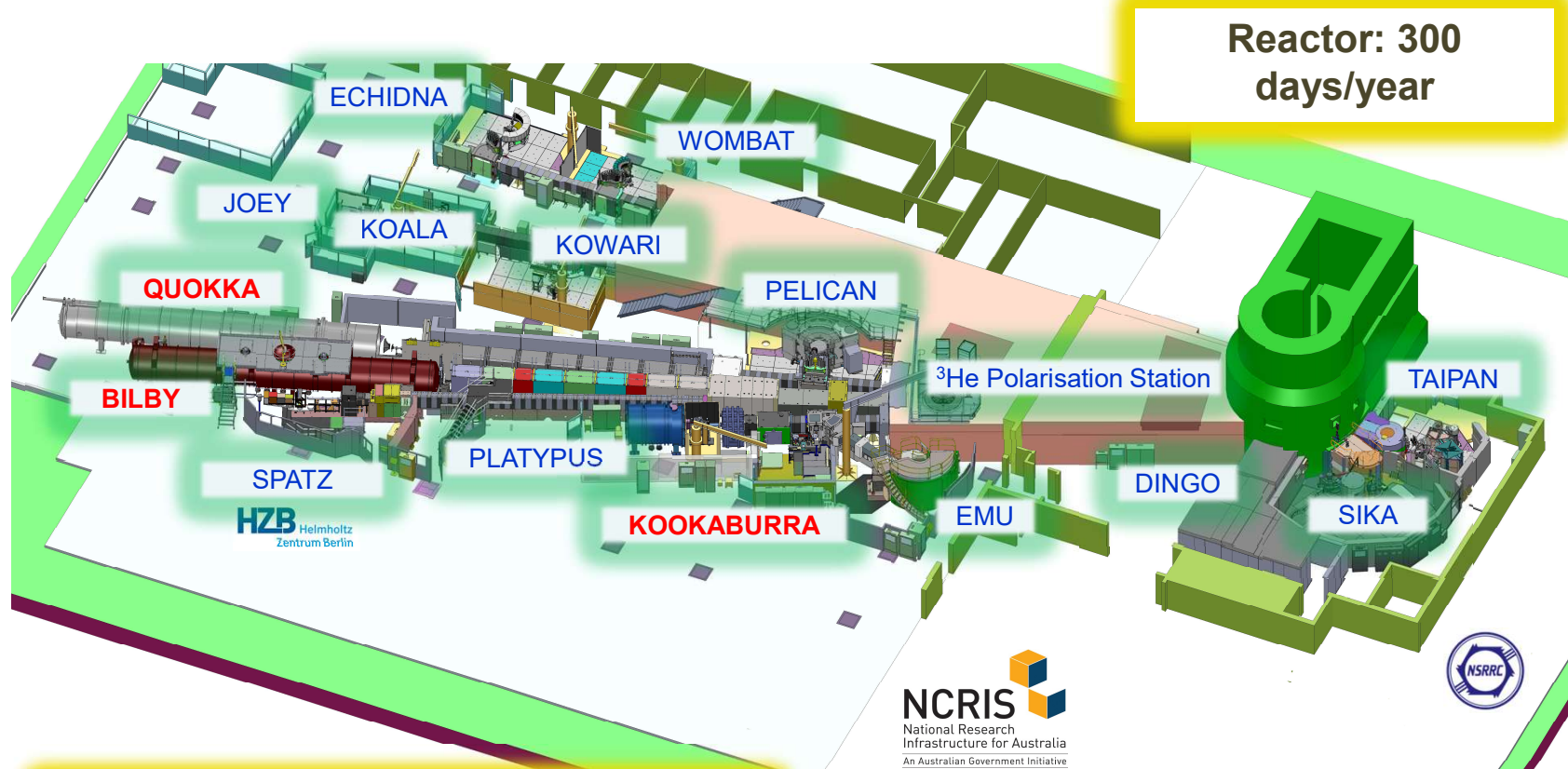


ACNS ANSTO: Mantid

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Small Angle Scattering Group manager
Bilby SANS Instrument Scientist

Australian Centre for Neutron Scattering



15 Neutron Beam Instruments
SAXS & X-ray Reflectometry
PPMS & Ellipsometry

ACNS: data reduction software

Single crystal diffraction

Koala

The LaueG software suite + SCILAB software package

Powder diffraction

Wombat

Gumtree and Python scripts for some samples, but more routinely uses LAMP

Echidna

Gumtree + Python scripts (<https://github.com/Gumtree/nbi-scripts>)

Strain Scanner

Kowari

Gumtree scripts

Imaging

Dingo

Pydingo, in-house package

Reflectometry

Platypus and Spatz

refnx <https://github.com/refnx/refnx>

Nelson, A.R.J. & Prescott, S.W. (2019). J. Appl. Cryst. 52, <https://doi.org/10.1107/S1600576718017296>

Bilby: ToF & monochromatic

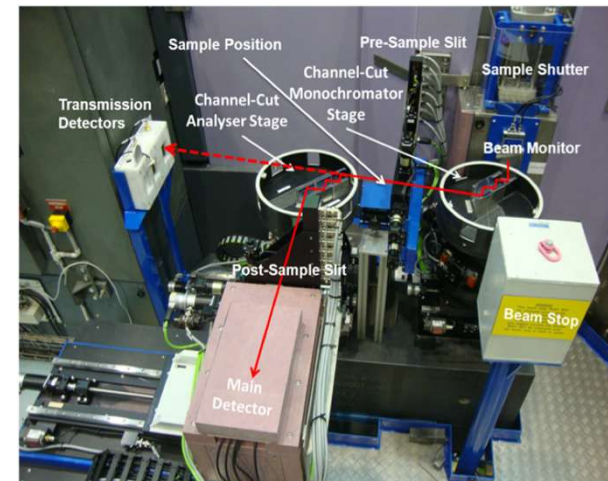
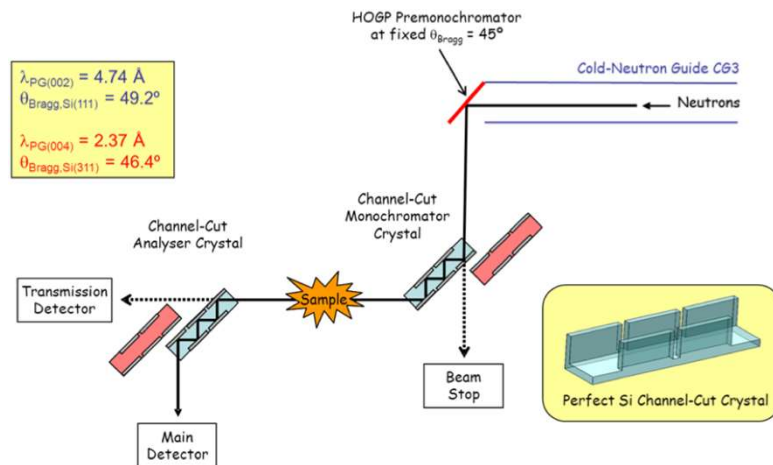
- Mantid Repo: main reducer
- https://github.com/hortica/Mantid_Bilby

NO User Interface, csv files as input



Kookaburra Mantid – local use

- Local – possibly valuable for all – thinking to upload to the Mantid repo (*contact us for details*)
 - De-smearing
 - Interpolation
 - Reading any random ASCII data



Reference: Rehm, C.; de Campo, L.; Brûlé, A.; Darmann, F.; Bartsch, F.; Berry, A., Design and performance of the variable-wavelength Bonse–Hart ultra-small-angle neutron scattering diffractometer KOOKABURRA at ANSTO. Journal of Applied Crystallography 2018, 51 (1), 1-8.

Inelastic spectroscopy Pelican

Cold-Neutron Time-of-Flight Spectrometer

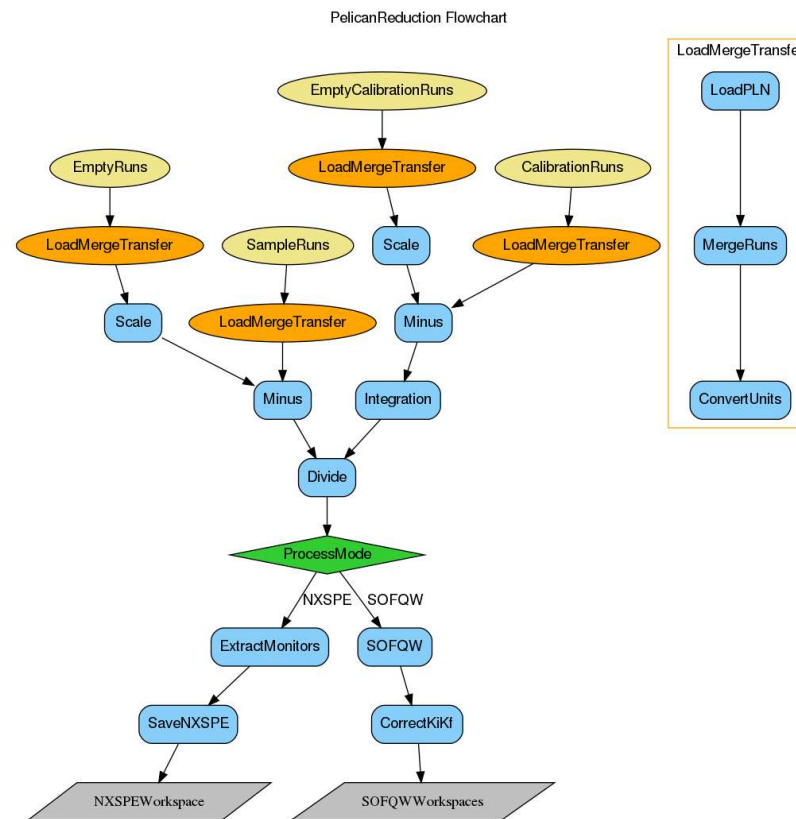
Energy resolution:
65 μeV (6 $\text{\AA}$), 135 μeV (4.69 $\text{\AA}$), 800 μeV (2.345 $\text{\AA}$)

<https://docs.mantidproject.org/v6.1.0/algorithms/PelicanReduction-v1.html>



Inelastic spectroscopy Pelican

- Mantid currently used on Pelican for approx. 70 % of data reduction.
 - All preliminary reduction for single crystal experiments performed with Mantid.
 - Approx 50 % of the powder experiments are performed with Mantid.
 - Some things such as fast Fourier transform to the time domain only implemented in Mantid on Pelican.



Inelastic spectroscopy Pelican

- LHS powder reduction.
- RHS single crystal processing (writes nxspe files).

PelicanReduction input dialog

Performs an inelastic energy transfer reduction for ANSTO Pelican geometry data.

SampleRuns	99902-99910	⌚
EmptyRuns	99996-100010	⌚
ScaleEmptyRuns	1	
CalibrationRuns	100020-100029	⌚
EmptyCalibrationRuns		
EnergyTransfer	-10,0.06,3	⌚
MomentumTransfer	0.2,0.1,2.4	⌚
Processing	SOFQW3-NormalisedPolygon	⌚
	☐ LambdaOnTwoMode	
	☐ FrameOverlap	
	☒ CalibrateTOF	⌚
TOFCorrection		
AnalyseTubes		
MaxEnergyGain		
OutputWorkspace	test_1p5K_Kate	⌚
ScratchFolder	C:/Data/Becky_fuller/Kate_data	Browse ⌚
	☐ KeepIntermediateWorkspaces	
ConfigurationFile	C:/Data/Becky_fuller/pelican_2.ini	Browse ⌚

? Keep Open ☐ Run Close

PelicanCrystalProcessing input dialog

Performs crystal processing for ANSTO Pelican data.

SampleRuns	108759-108880	⌚
EmptyRuns		
ScaleEmptyRuns	0	⌚
CalibrationRuns		
EmptyCalibrationRuns		
EnergyTransfer	-9,0.02,9	⌚
MomentumTransfer	0,0.05,6	⌚
	☒ LambdaOnTwoMode	⌚
	☐ FrameOverlap	
	☒ CalibrateTOF	⌚
TOFCorrection		
AnalyseTubes		
MaxEnergyGain		
	☒ FixedDetector	
OutputFolder	C:/Data/Robinson/no_bkg	Browse ⌚
ScratchFolder	C:/Data/Robinson/P9851_data	Browse ⌚
ConfigurationFile	C:/Data/Robinson/pelican.ini	Browse ⌚
	☐ KeepReducedWorkspace	

? Keep Open ☐ Run Close

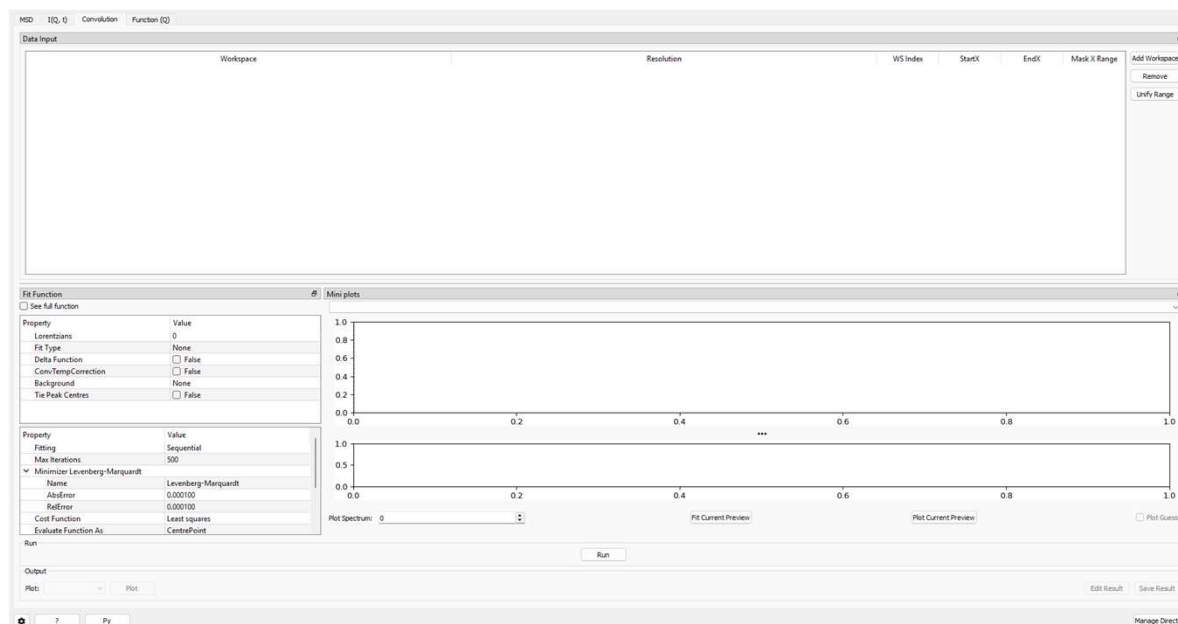
Inelastic spectroscopy Pelican

- Typical Pelican python script.
- These scripts are the preferred method of reduction as it ensures reproducibility.

```
1 from mantid.simpleapi import *
2 import matplotlib.pyplot as plt
3 import numpy as np
4
5 def pelican_reduction(samples, output):
6     PelicanReduction(SampleRuns=samples,
7                      EnergyTransfer='-150,0.03,3',
8                      MomentumTransfer='0,0.01,8',
9                      Processing='SOFQW3-NormalisedPolygon',
10                     CalibrateTOF=True, OutputWorkspace=output,
11                     ScratchFolder='H:/pelican_dav1_D_drive/lambda/anatoliy',
12                     KeepIntermediateWorkspaces=True,
13                     ConfigurationFile='C:/pelican_mantid/pelican_work_cycle_range.ini')
14
15
16 #####EC
17
18 pelican_reduction('124314-124431', '150k_200Hz')
19 pelican_reduction('124432-124550', '150k_100Hz')
20 pelican_reduction('124551-124669', '200k_100Hz')
21 pelican_reduction('124670-124788', '100k_100Hz')
22 pelican_reduction('124789-124907', '225k_100Hz')
23 pelican_reduction('124908-125026', '250k_100Hz')
24 pelican_reduction('125027-125144', '300k_100Hz')
25 pelican_reduction('125146-125240', '320k_100Hz')
26 #pelican_reduction('121405-121408', '150k_test')
27
28
29 #ComputeIncoherentDOS(InputWorkspace='70k_test_qw3_2D', Temperature=70, EnergyBinning='-100,0.5,20', OutputWorkspace='70k_test_gdos')
30 ComputeIncoherentDOS(InputWorkspace='150k_200Hz_qw3_2D', Temperature=150, EnergyBinning='-150,0.3,20', OutputWorkspace='150k_200Hz_gdos')
31 ComputeIncoherentDOS(InputWorkspace='150k_100Hz_qw3_2D', Temperature=150, EnergyBinning='-60,0.3,20', OutputWorkspace='150k_100Hz_gdos')
32 ComputeIncoherentDOS(InputWorkspace='200k_100Hz_qw3_2D', Temperature=200, EnergyBinning='-60,0.3,20', OutputWorkspace='200k_100Hz_gdos')
33 ComputeIncoherentDOS(InputWorkspace='100k_100Hz_qw3_2D', Temperature=100, EnergyBinning='-50,0.3,20', OutputWorkspace='100k_100Hz_gdos')
34 ComputeIncoherentDOS(InputWorkspace='225k_100Hz_qw3_2D', Temperature=225, EnergyBinning='-150,0.3,20', OutputWorkspace='225k_100Hz_gdos')
35 ComputeIncoherentDOS(InputWorkspace='250k_100Hz_qw3_2D', Temperature=250, EnergyBinning='-150,0.3,20', OutputWorkspace='250k_100Hz_gdos')
36 ComputeIncoherentDOS(InputWorkspace='300k_100Hz_qw3_2D', Temperature=300, EnergyBinning='-150,0.3,20', OutputWorkspace='300k_100Hz_gdos')
37 ComputeIncoherentDOS(InputWorkspace='320k_100Hz_qw3_2D', Temperature=320, EnergyBinning='-150,0.3,20', OutputWorkspace='320k_100Hz_gdos')
38
39 #####DMC
40 pelican_reduction('125265', 'DMC_300k_100Hz')
41
42 pelican_reduction('125278-125396', 'DMC_100k_100Hz')
43 pelican_reduction('125397-125515', 'DMC_150k_100Hz')
44 pelican_reduction('125516-125634', 'DMC_200k_100Hz')
45 pelican_reduction('125635-125753', 'DMC_225k_100Hz')
46 pelican_reduction('125754-125872', 'DMC_250k_100Hz')
47 pelican_reduction('125873-126014', 'DMC_300k_full_100Hz')
48
49 ComputeIncoherentDOS(InputWorkspace='DMC_100k_100Hz_qw3_2D', Temperature=100, EnergyBinning='-150,0.3,20', OutputWorkspace='DMC_100k_100Hz_gdos')
50 ComputeIncoherentDOS(InputWorkspace='DMC_150k_100Hz_qw3_2D', Temperature=150, EnergyBinning='-150,0.3,20', OutputWorkspace='DMC_150k_100Hz_gdos')
```

Inelastic spectroscopy Pelican: fitting – positive feedback

- We have been using the QENS fit tool.
 - There are some really useful features (eg fitting results>EISF).
 - The visualisation isn't always the best (eg squashed mini plots).
 - Large number of output workspaces gets confusing.



Inelastic spectroscopy Pelican: other software's used

- LAMP (Legacy. For powder work this is faster – if you know how to use it).
- Horace (both matlab and Python). Single crystal processing.
- DAVE. Often pass Mantid output to DAVE as users prefer the fitting options available.

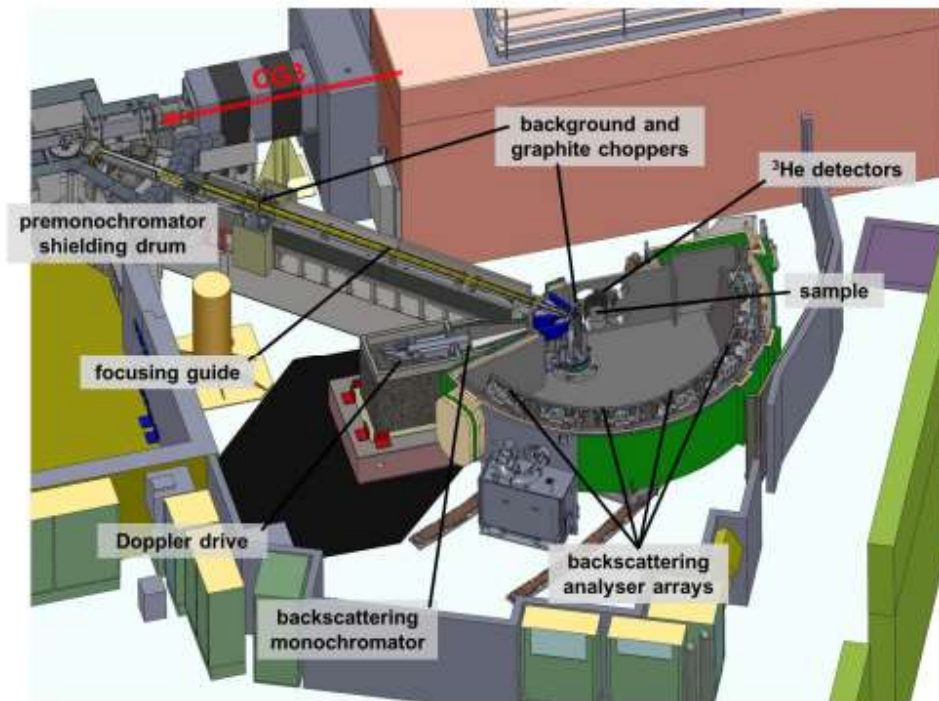
Inelastic spectroscopy Pelican: Future development?

- If we could use Horace (python version) within the Mantid python environment.
- That would allow us to process data straight from event data through to a 4D SQW file in one platform.

Emu Mantid

Cold-Neutron Backscattering Spectrometer

<https://docs.mantidproject.org/v6.7.0/algorithms/InelasticEMUauReduction-v1.html>



Emu – Data Reduction

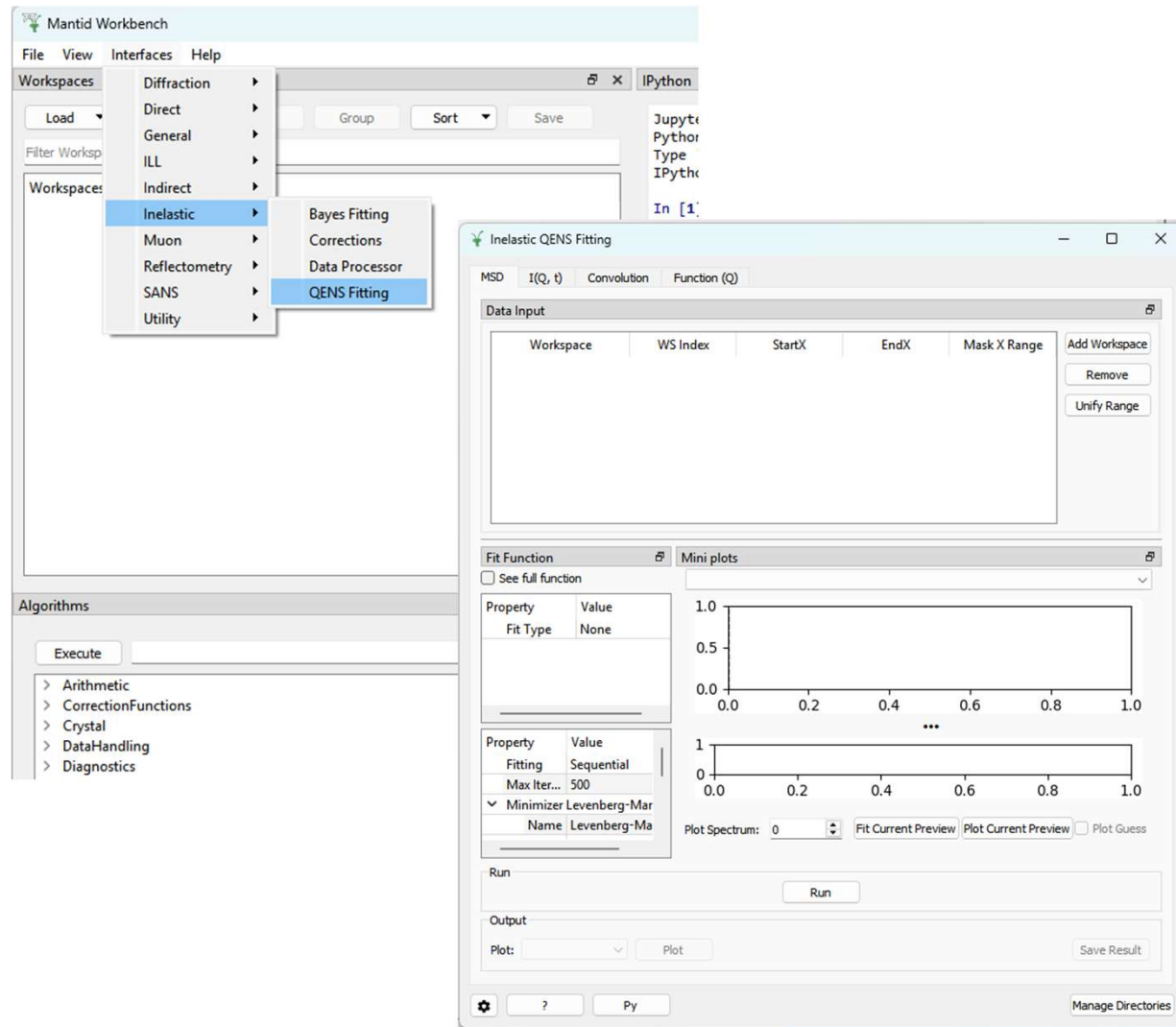
The screenshot displays the Mantid Workbench interface, which is used for neutron data reduction. The interface is divided into several panels:

- Workspaces:** A list of available workspaces on the left. The workspace `35034-35045_vanadium_30mm_300K_Q_cal` is selected.
- Algorithms:** A list of algorithms on the left. The `InelasticEMUauReduction` algorithm is selected.
- InelasticEMUauReduction input dialog:** A dialog box for configuring the inelastic reduction. It includes fields for `SampleRuns` (35034-35045), `BackgroundRuns` (35034-35045), `CalibrationRuns` (35034-35045), `BackgroundCalibrationRuns` (35219-35240), `IncidentSpectrumRuns` (35034-35045), `SpectrumAxis` (Q), `SampleTransmissionFactor` (0.85), `CalibrationTransmissionFactor` (0.85), `OutputWorkspace` (35034-35045_Vanadium_300K), `ScratchFolder` (Z:/Calibration/QKB_bkg_Quartz/scratch), `ConfigurationFile` (QKB_bkg_Quartz/emu-mantid-elastic.ini), and `UseFractionalMap` (checked).
- ElasticEMUauReduction input dialog:** A dialog box for configuring the elastic reduction. It includes fields for `SampleRuns` (35879:*), `BackgroundRuns` (35910), `CalibrationRuns` (35923), `BackgroundCalibrationRuns` (35923), `SpectrumAxis` (Q), `SampleTransmissionFactor` (1), `CalibrationTransmissionFactor` (1), `ScanParameter` (T152), `ReferenceRange` (202-205), `OutputWorkspace` (35879_S1_heating), `ScratchFolder` (Z:/USER/Willy_hydrogel/P19650/Scratch), `ConfigurationFile` (hydrogel/P19650/emu-mantid-elastic.ini), and `UseFractionalMap` (checked).
- Plots:** Two plots are shown. The top plot, titled `35034-35045_vanadium_30mm_300K_Q_cal_1D`, shows a sharp peak at approximately 0.01 meV. The bottom plot, titled `35825_10pc_GelMA_D2O_heating_Q_bkg_cal_bm_2D`, shows a series of curves representing the heating of GelMA-D2O at different temperatures (from 0.32 to 1.72 K).

Two blue starburst shapes are overlaid on the image, labeled **Inelastic** and **Elastic**, indicating the type of data reduction being performed.

... more Functionality needed – maybe cross-Institutional

- consecutive data analysis/fitting
- applicable to spectrometer at various neutron research facilities
- streamline fitting procedures
- standardised data format (loader for data analysis)



ACNS, ANSTO – summary – various inputs – coding / science / mix

- Computing group: Geish Miladinovic (<0.3 FT)
 - **Inelastic Pelican** Richard Mole, Dehong Yu
 - **Backscattering Emu** Alice Klapproth, Nicolas de Souza
 - **SANS Bilby** Anna Sokolova, Liliana de Campo
 - **USANS Kookaburra** Rainer Mittelbach, Liliana de Campo, Jitendra Mata