ACNS ANSTO: Mantid

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Small Angle Scattering Group manager
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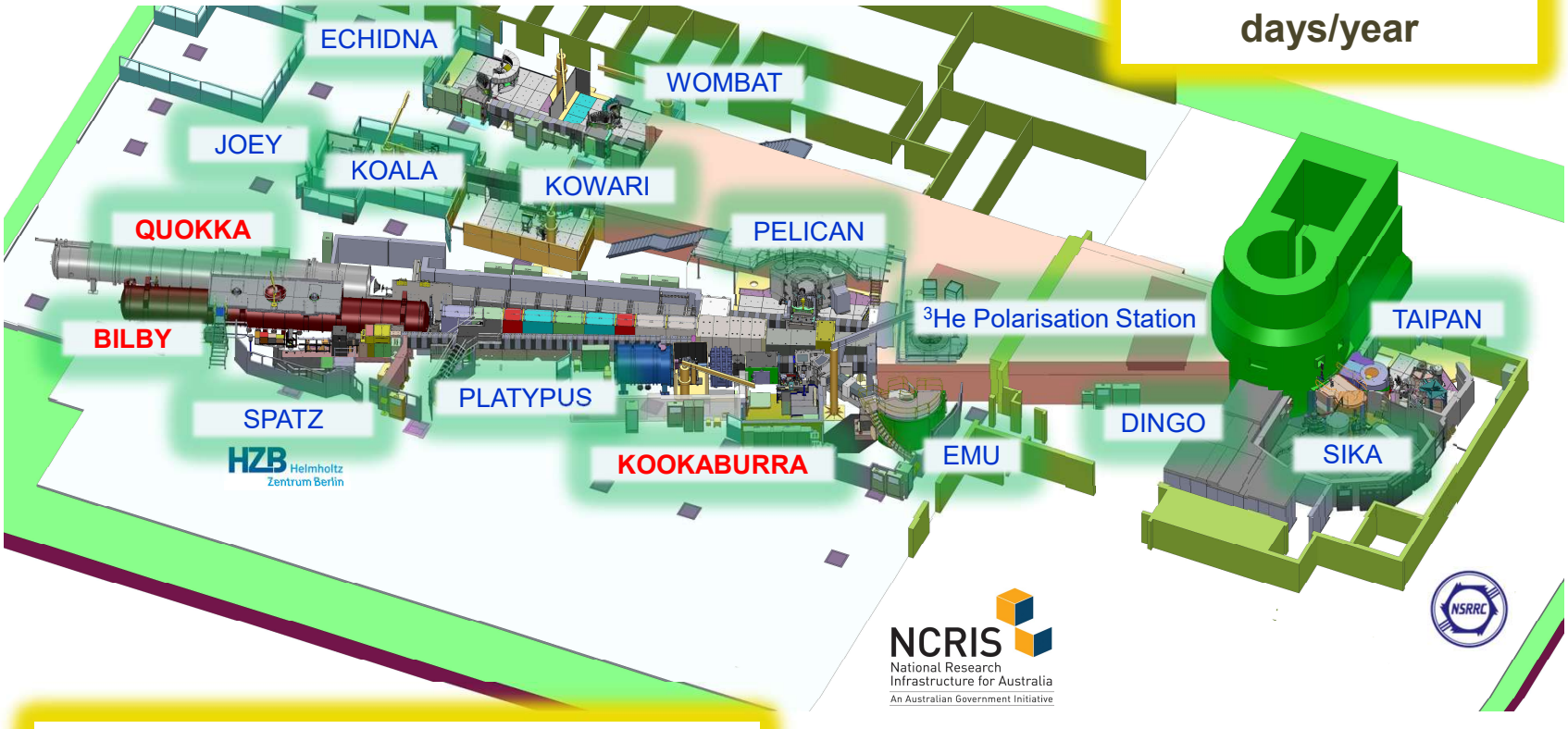
ANSTO

Australian Centre for Neutron Scattering

Reactor: 300 days/year



15 Neutron Beam Instruments

SAXS & X-ray Reflectometry

PPMS & Ellipsometry

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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

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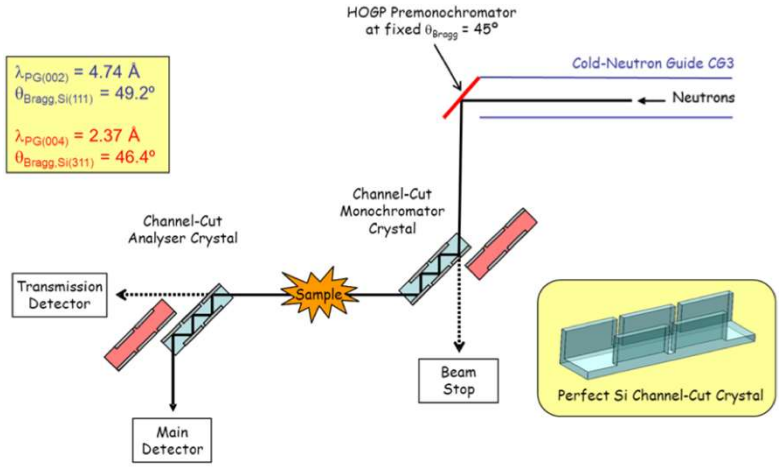
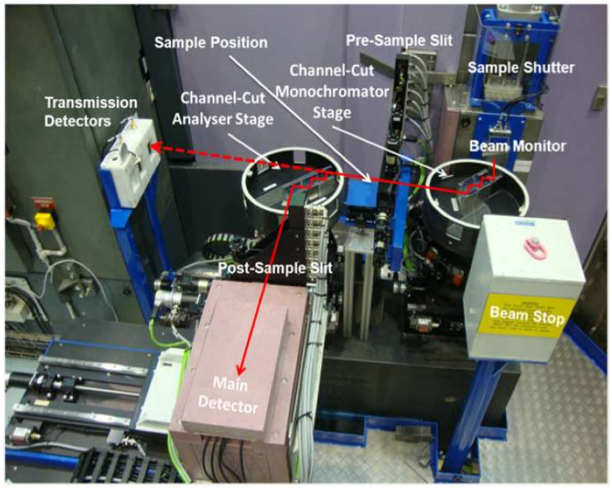
Kookaburra Mantid – local use

- 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 Å), 135 µeV (4.69 Å), 800 µeV (2.345 Å)

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

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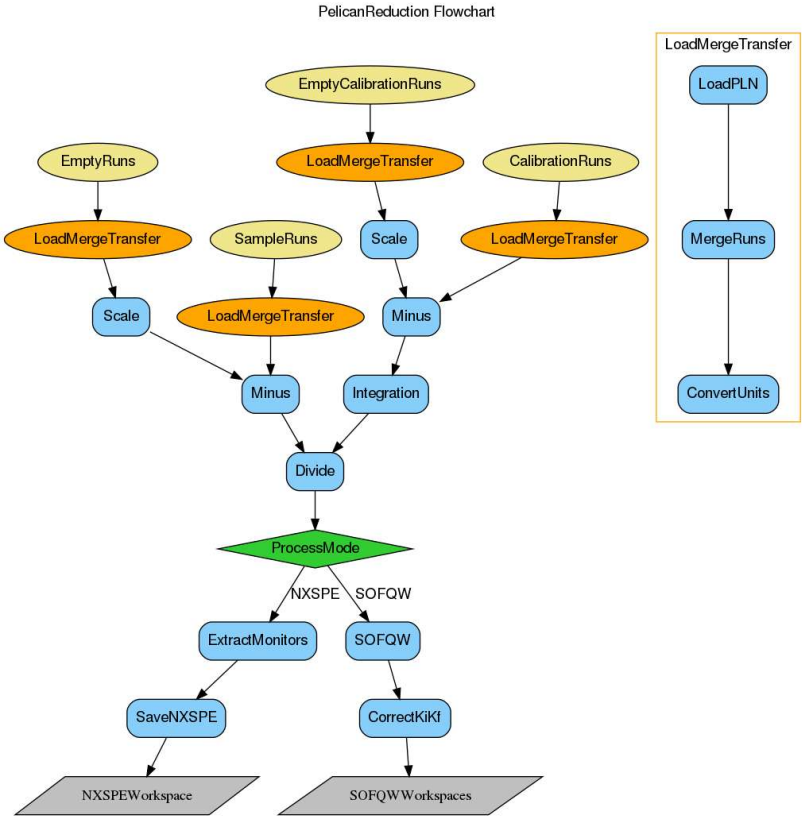
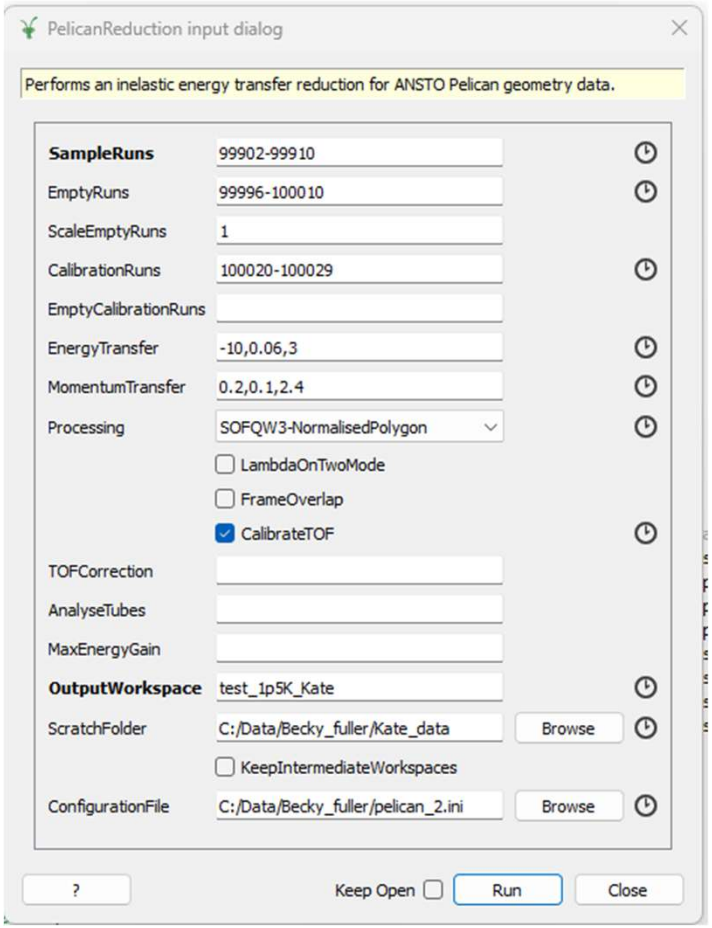
Inelastic spectroscopy Pelican

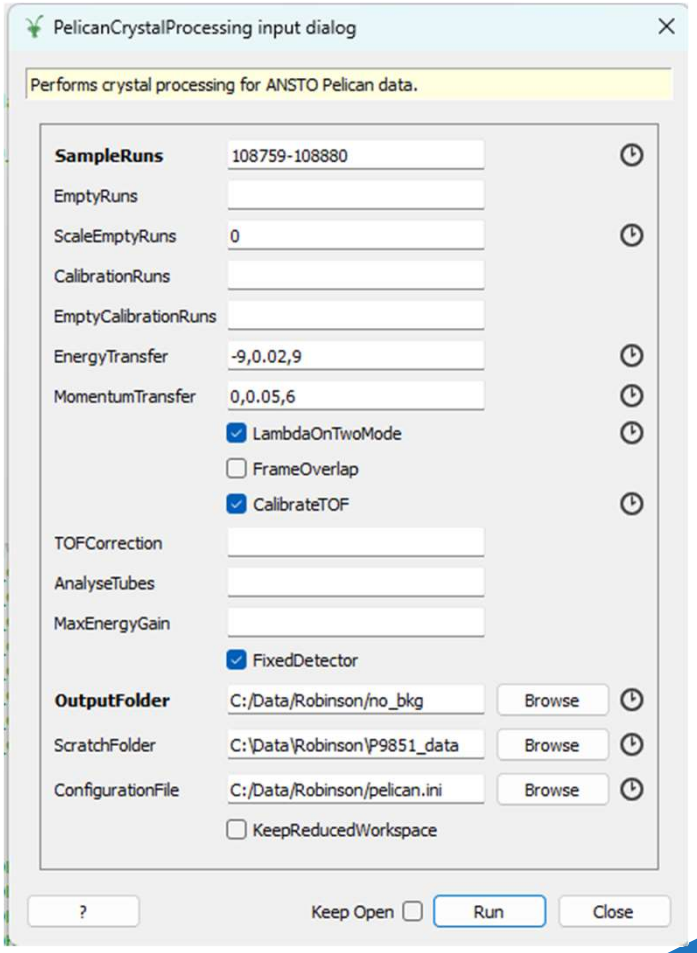
- Mantid currently used on Pelican for approx. 70 % of data reduction.
  - All preliminary reduction for single crystal experiments performed with Mantid.
  - Approx 50 % of the powder experiments are performed with Mantid.
  - Some things such as fast Fourier transform to the time domain only implemented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



Inelastic spectroscopy Pelican

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





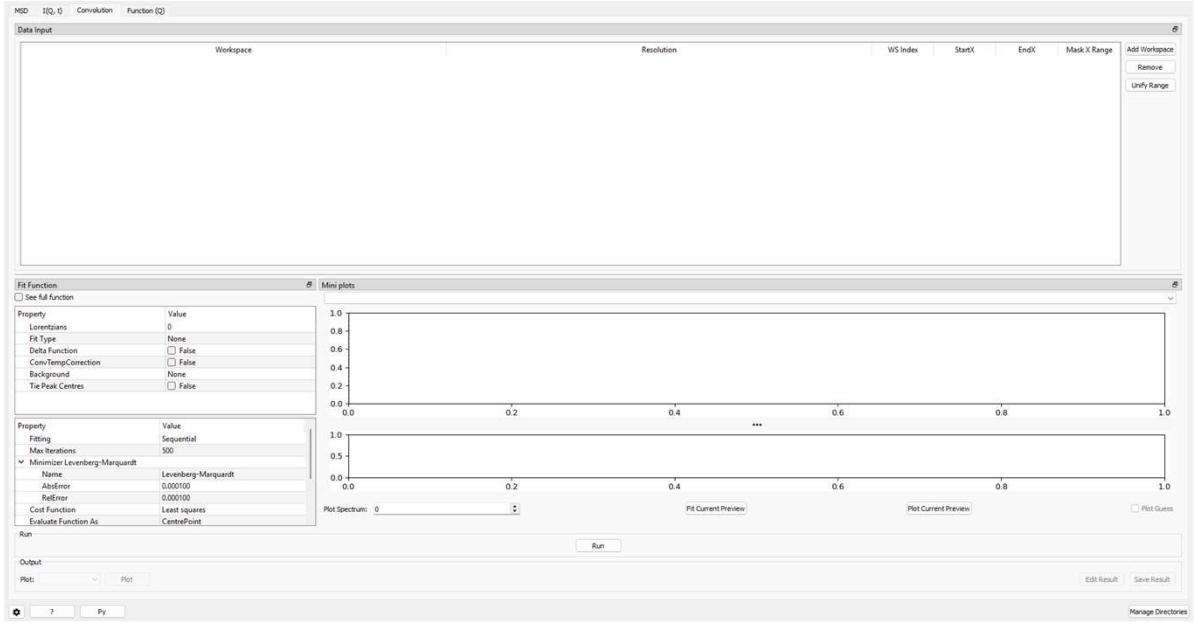
Inelastic spectroscopy Pelican

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

```python
from mantid.simpleapi import *
import matplotlib.pyplot as plt
import numpy as np

def pelican_reduction(samples, output):
    PelicanReduction(SampleRuns=samples,
    EnergyTransfer='-150,0.03,3',
    MomentumTransfer='0,0.01,8',
    Processing='SOFQW3-NormalisedPolygon',
    CalibrateTOF=True, OutputWorkspace=output,
    ScratchFolder='H:/pelican_dav1_D_drive/lambda/anatoliy',
    KeepIntermediateWorkspaces=True,
    ConfigurationFile='C:/pelican_mantid/pelican_work_cycle_range.ini')


######EC

pelican_reduction('124314-124431', '150k_200Hz')
pelican_reduction('124432-124550', '150k_100Hz')
pelican_reduction('124551-124669', '200k_100Hz')
pelican_reduction('124670-124788', '100k_100Hz')
pelican_reduction('124789-124907', '225k_100Hz')
pelican_reduction('124908-125026', '250k_100Hz')
pelican_reduction('125027-125144', '300k_100Hz')
pelican_reduction('125146-125240', '320k_100Hz')
#pelican_reduction('121405-121408', '150k_test')


#ComputeIncoherentDOS(InputWorkspace='70k_test_qw3_2D', Temperature=70, EnergyBinning='-100,0.5,20', OutputWorkspace='70k_test_gdos')
ComputeIncoherentDOS(InputWorkspace='150k_200Hz_qw3_2D', Temperature=150, EnergyBinning='-150,0.3,20', OutputWorkspace='150k_200Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='150k_100Hz_qw3_2D', Temperature=150, EnergyBinning='-60,0.3,20', OutputWorkspace='150k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='200k_100Hz_qw3_2D', Temperature=200, EnergyBinning='-60,0.3,20', OutputWorkspace='200k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='100k_100Hz_qw3_2D', Temperature=100, EnergyBinning='-50,0.3,20', OutputWorkspace='100k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='225k_100Hz_qw3_2D', Temperature=225, EnergyBinning='-150,0.3,20', OutputWorkspace='225k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='250k_100Hz_qw3_2D', Temperature=250, EnergyBinning='-150,0.3,20', OutputWorkspace='250k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='300k_100Hz_qw3_2D', Temperature=300, EnergyBinning='-150,0.3,20', OutputWorkspace='300k_100Hz_gdos')
ComputeIncoherentDOS(InputWorkspace='320k_100Hz_qw3_2D', Temperature=320, EnergyBinning='-150,0.3,20', OutputWorkspace='320k_100Hz_gdos')

#####DMC
pelican_reduction('125265', 'DMC_300k_100Hz')

pelican_reduction('125278-125396', 'DMC_100k_100Hz')
pelican_reduction('125397-125515', 'DMC_150k_100Hz')
pelican_reduction('125516-125634', 'DMC_200k_100Hz')
pelican_reduction('125635-125753', 'DMC_225k_100Hz')
pelican_reduction('125754-125872', 'DMC_250k_100Hz')
pelican_reduction('125873-126014', 'DMC_300k_full_100Hz')

ComputeIncoherentDOS(InputWorkspace='DMC_100k_100Hz_qw3_2D', Temperature=100, EnergyBinning='-150,0.3,20', OutputWorkspace='DMC_100k_100Hz_gdos')
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.



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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.

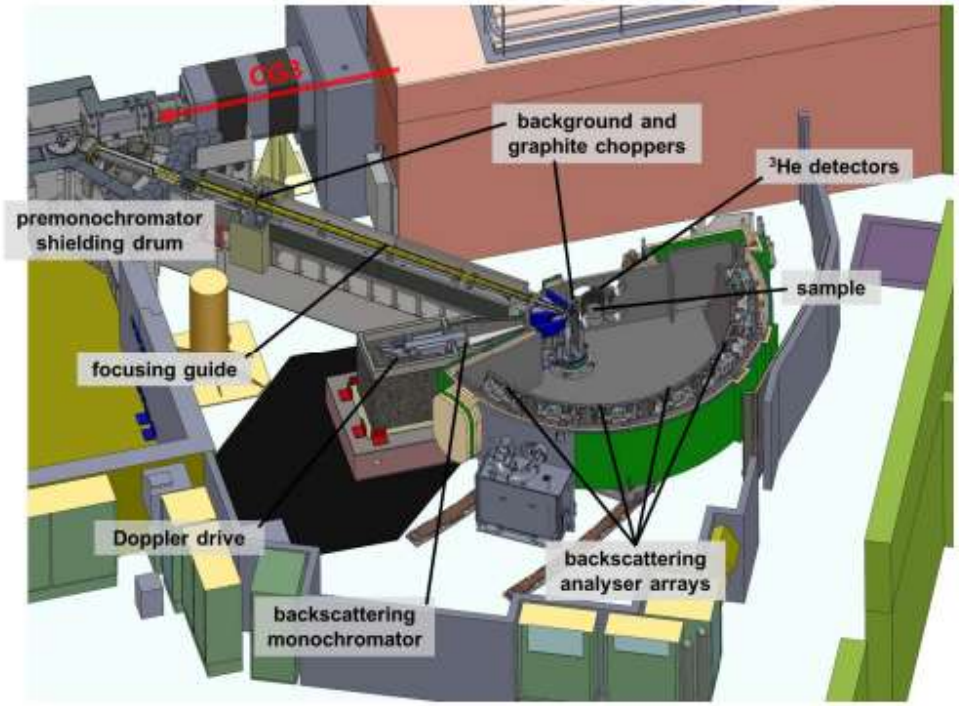
Inelastic spectroscopy Pelican: Future development?

- 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



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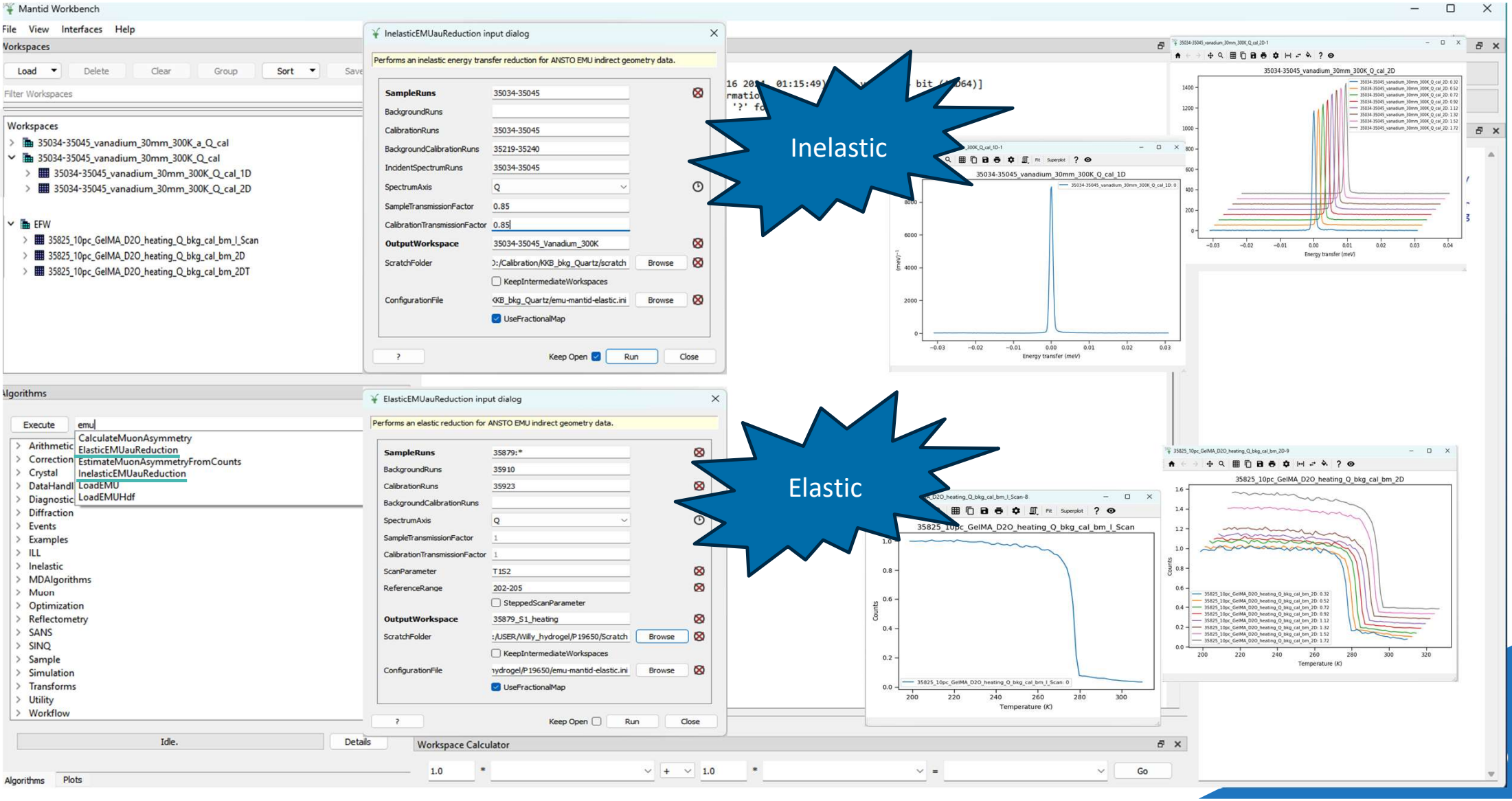
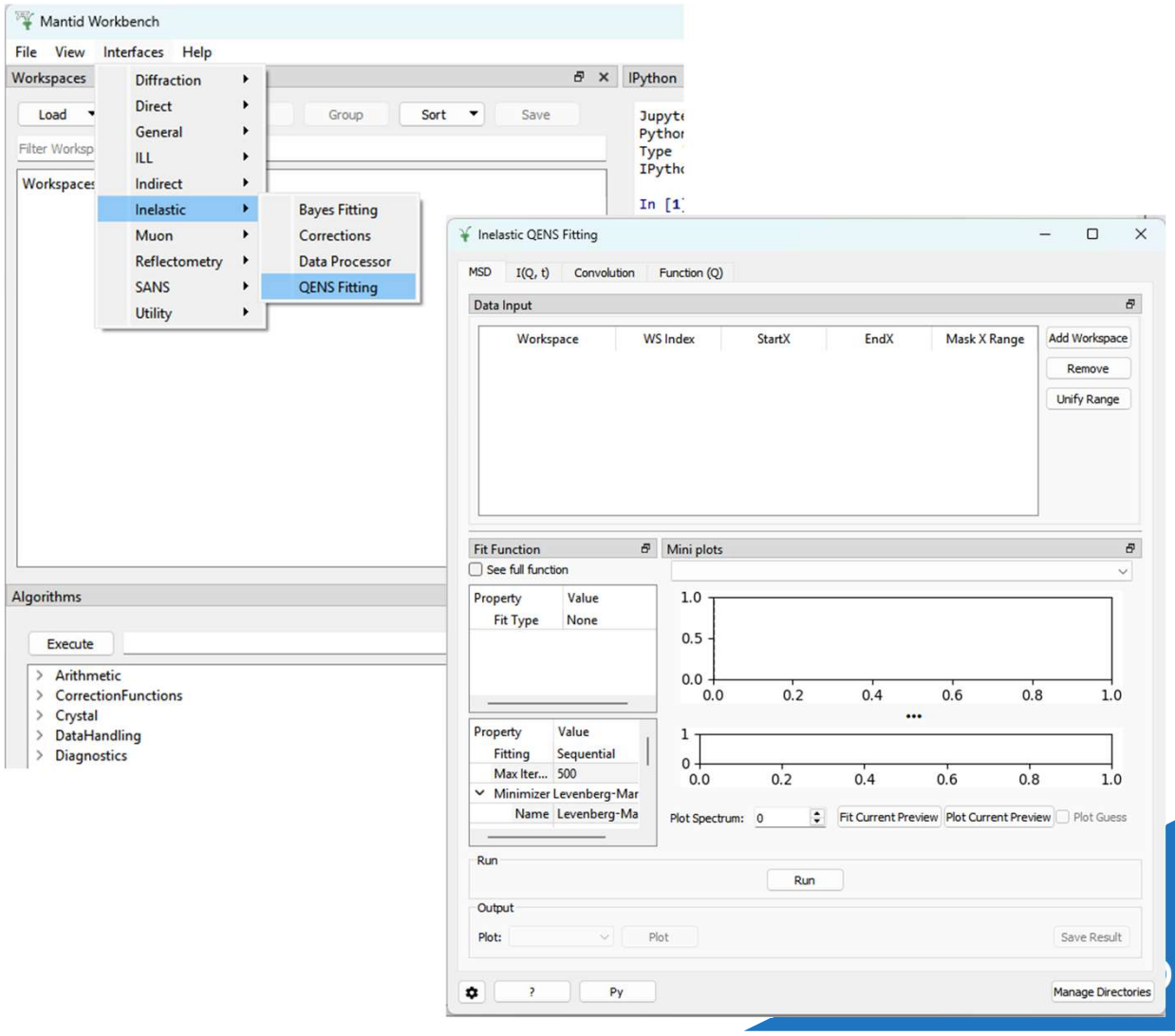
Emu – Data Reduction



… 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