Polarized diffraction and spectroscopy data reduction in Mantid

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Introduction

Polarized neutrons experiments are the only technique allowing to analyze individual contributions from nuclear-coherent, incoherent, and magnetic components of neutron scattering cross-section necessary to study, among others, properties of paramagnetic materials.

The new reduction workflow supports monochromatic and single-crystal diffraction, as well as time-of-flight measurements, using Z-only, 6-point, or 10-point component-separation methods. Extensive examples with all relevant mathematics and workflow diagrams are available in *Data reduction for D7 instrument at the ILL* documentation accessible via Mantid project website.
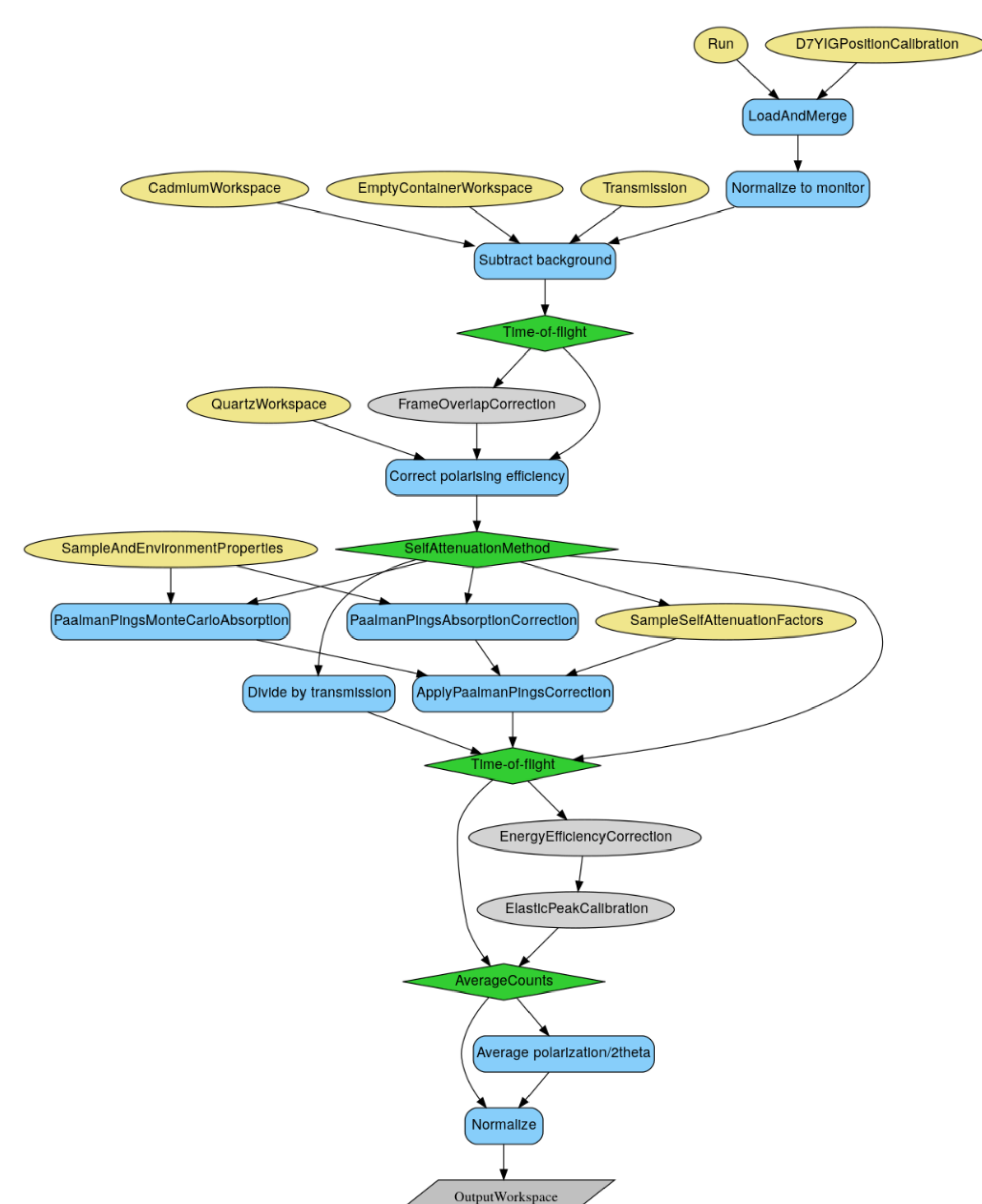
2. D7 instrument

- General-purpose diffuse scattering spectrometer, always polarised
- Wavelengths available: 3.1, 4.8, and 5.7 Å
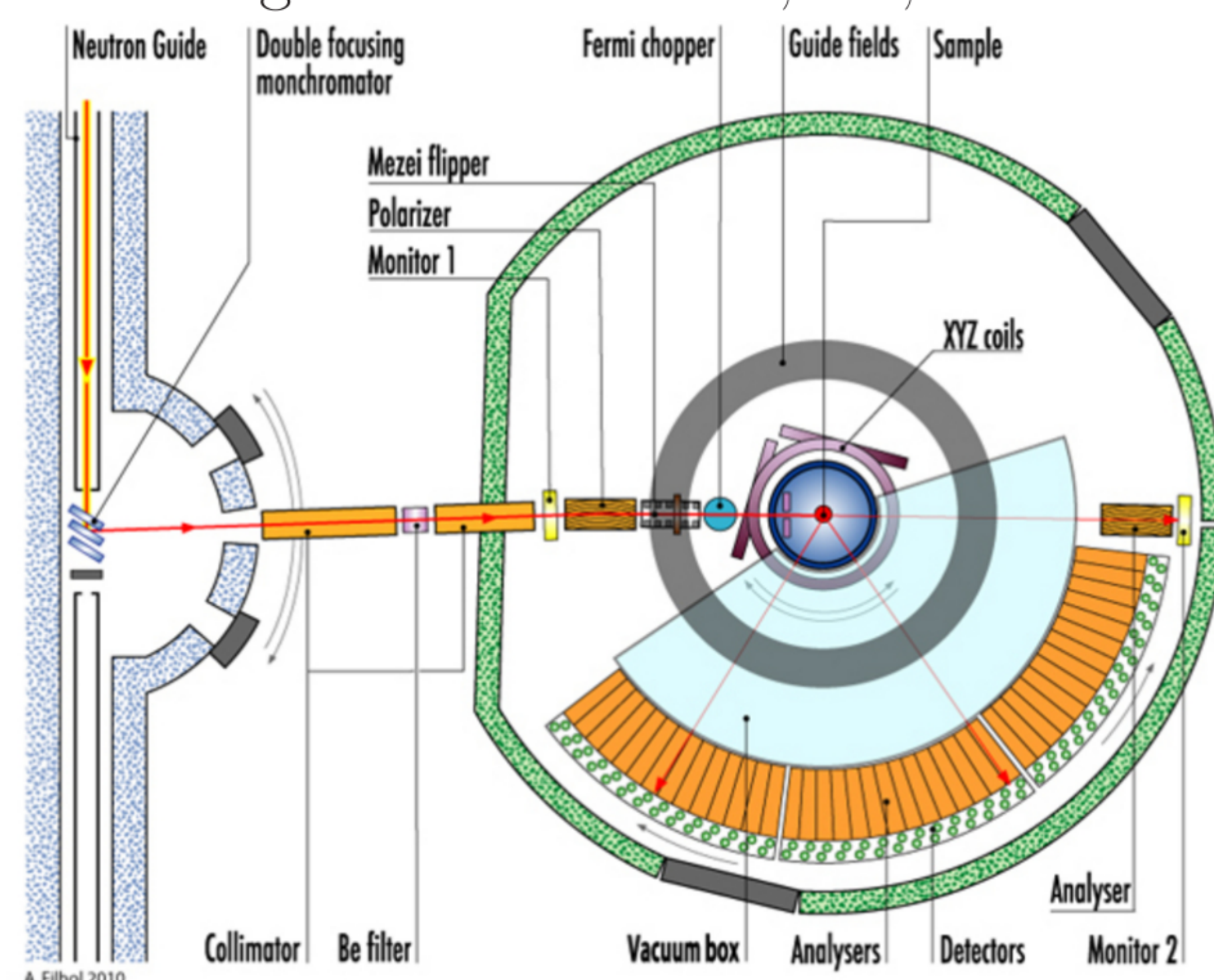
D7 instrument layout

## 3. Reduction workflow

Sample reduction workflow

4. YIG calibration

- Exact λ and bank positions need calibration after each λ change
- Calibration: 2θ scan of standard YIG sample measurement, well known d-spacing
- Peaks positioned fitted with Gaussians, compared to expected position
- Handled by bespoke Python algorithm D7YIGPositionCalibration
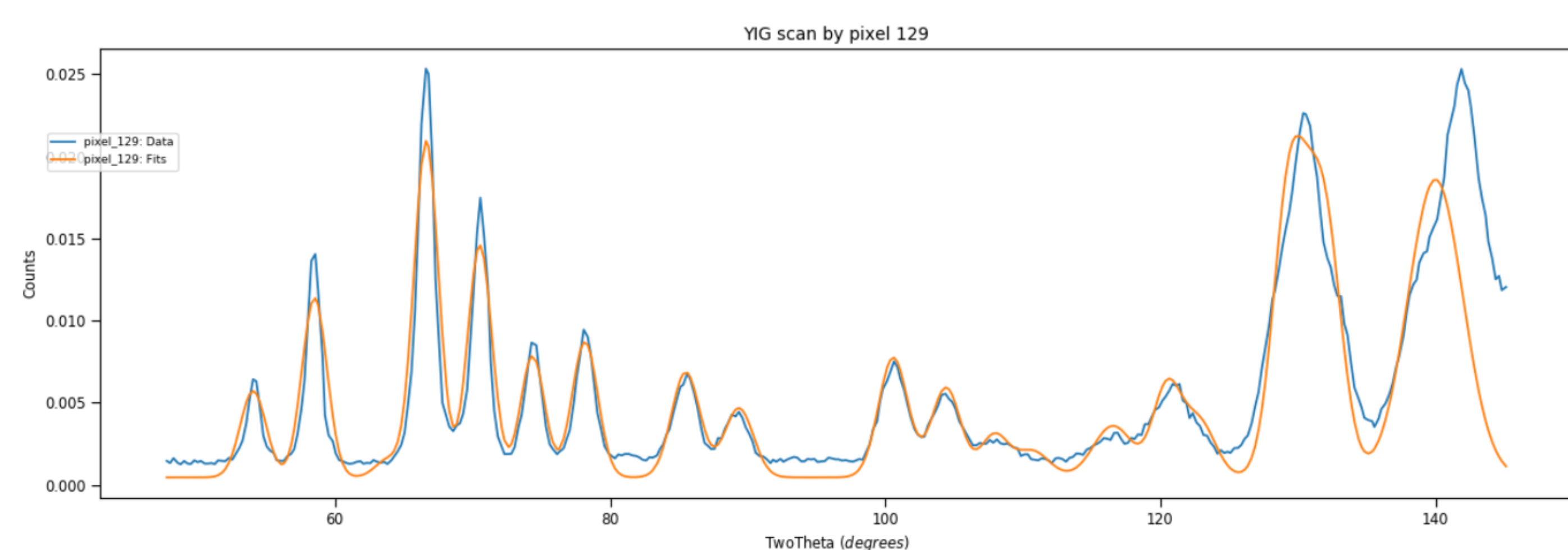
5. Polarised diffraction: powder and single crystal

- Reduction split in two stages: loading + corrections, and component separation + normalisation
- Loading handled by bespoke NeXus C++ loader: LoadILLPolarisedDiffraction
- Corrections: normalisation to monitor/time, background subtraction, polarisation correction, and self-attenuation handled by a Python algorithm PolDiffILLReduction
- Component separation (nuclear coherent, spin-incoherent, paramagnetic) and normalisation to vanadium, incoherent or paramagnetic cross-sections done in a Python algorithm D7AbsoluteCrossSections
- Single crystal reduction uses anisotropic magnetism separation according to Ref. [2]
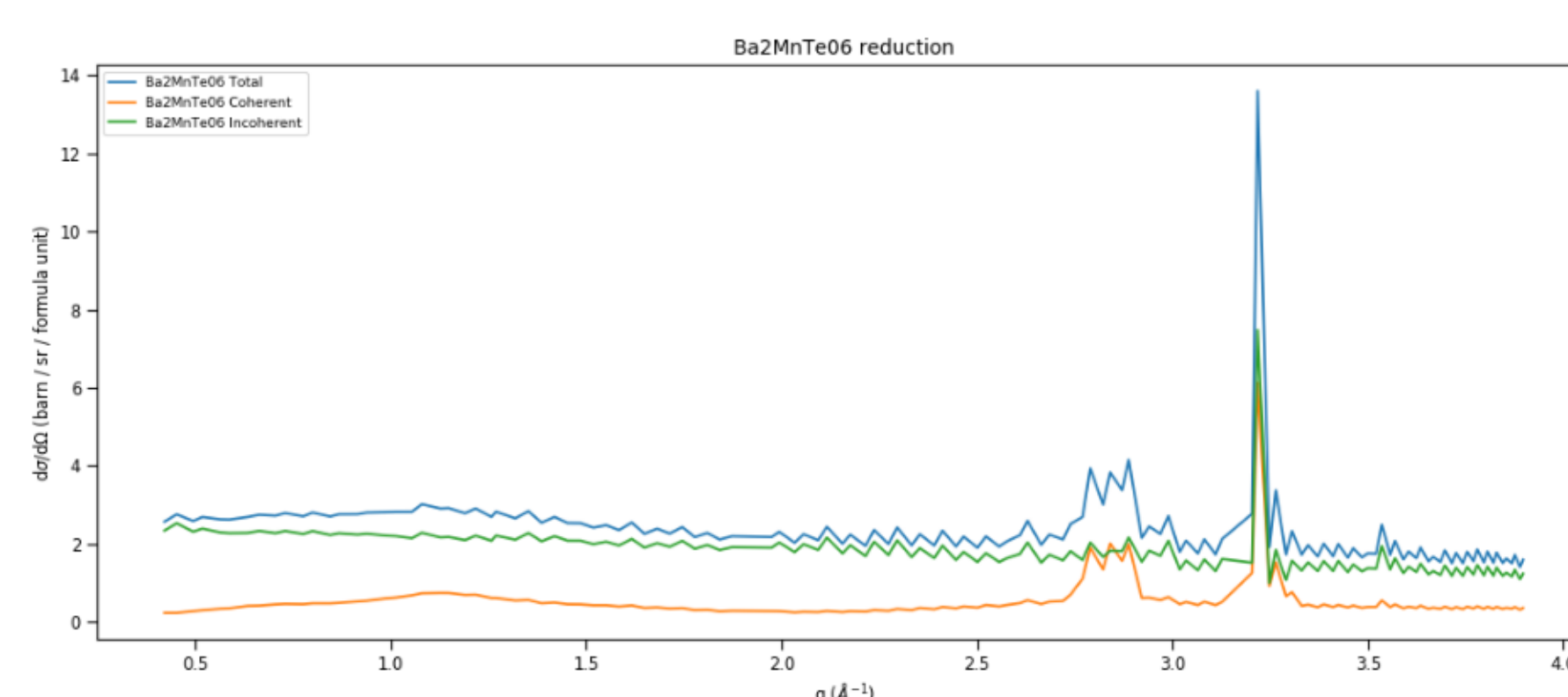
Ba2MnTeO6 powder sample cross-sections
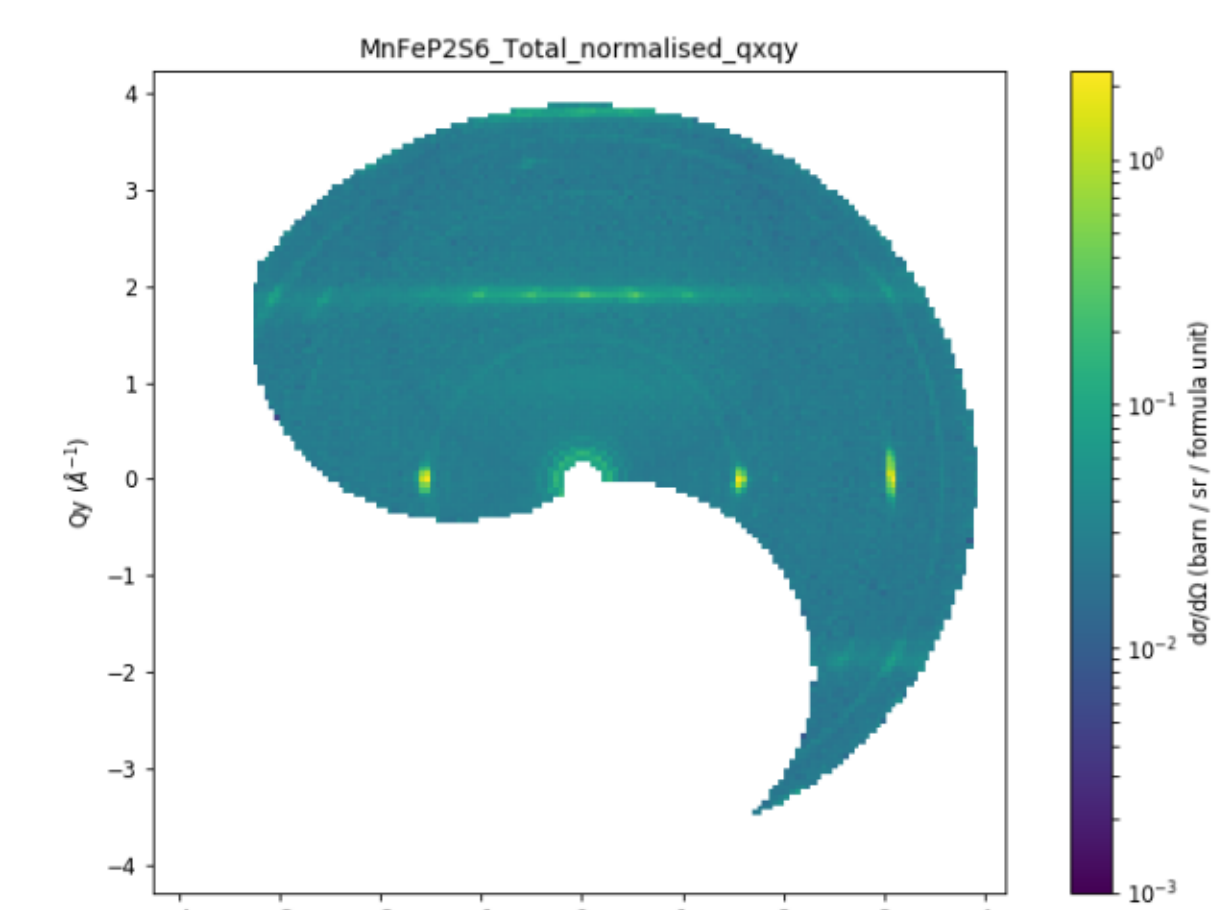
MnFeP2S6 single crystal total cross-section

6. Polarised spectroscopy

- Same algorithms are used for polarised spectroscopy
- Different corrections: time-dependent background, time-frame overlap, energy efficiency, and elastic peak calibration
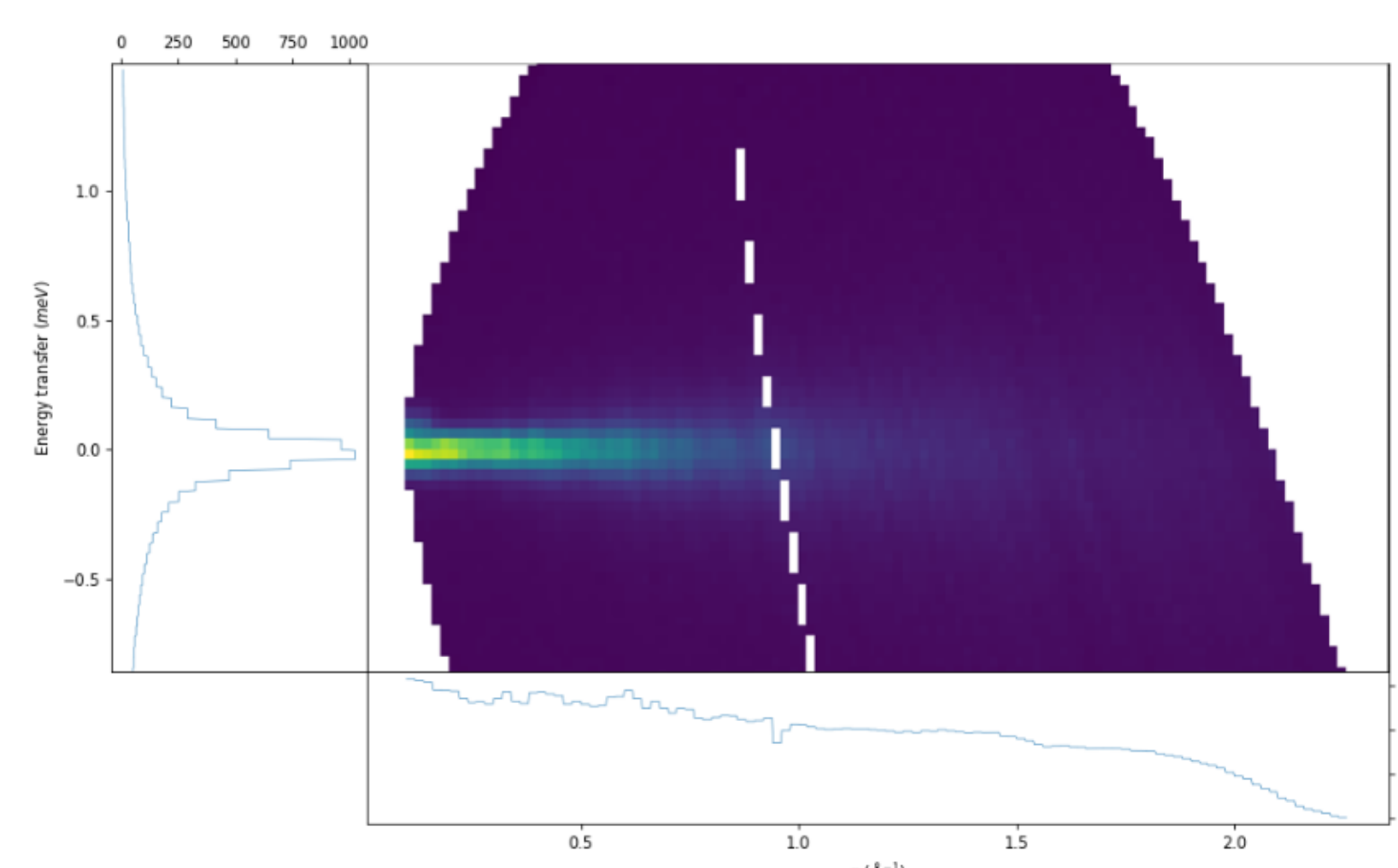
Total cross-section of water on ΔE - q plane

7. Conclusions

- A full data reduction implemented for D7.
- The package includes calibration, raw data loading and visualization, and reduction in absolute units.
- Code for D7 will be used as the base for data reduction of D3L and upgraded instrument D007.

References

[1] G. Ehlers, J. R. Stewart, A. R. Wildes, P. P. Deen, and K. H. Andersen. Generalization of the classical xyz-polarization analysis technique to out-of-plane and inelastic scattering. *Review of Scientific Instruments*, 2013.

[2] Werner Schweika. XYZ-polarisation analysis of diffuse magnetic neutron scattering from single crystals. *Journal of Physics: Conference Series*, 2010.