**Authors: Owen Arnold**

**Affiliations:** Tessella

**Preferred type of communication:** Oral

**Topics:** “Neutron Instrumentation, Optics, Sample Environment, Detectors and Software”

**Title (plain text only):** Visualisation and Analysis in Mantid for Single Crystal Neutron Diffraction

**Title (formatted text):** Visualisation and Analysis in Mantid for Single Crystal Neutron Diffraction

Large neutron scattering datasets are commonly collected at TOF sources, particularly for single crystal diffraction experiments. A full understanding of the materials of interest often requires the complete mapping of data in an n-dimensional manifold. Increasingly, and particularly in single crystal diffraction, the correct treatment of data as part of data reduction and analysis, for a range of techniques, involves the efficient and flexible processing of large n-dimensional datasets.

The Mantid1,2 framework, our extensible framework for neutron and muon data reduction and analysis, has been successfully deployed for use on a large range of instruments. An on-going area of development within that framework has been the development of tools to analyse and visualise n-dimensional data. This work has involved collaboration between ISIS at RAL, SNS at Oakridge and the ESS in Lund.

On the Analysis side, we have used a mixed team of instrument scientists and software engineers, to develop key features to solve complex problems within the data reduction. For example, providing efficient sparse data representation in n-dimensional space and allowing n-dimensional algorithms to operate on them. Recent work has been focused on peak integration, for which we have developed new algorithms based on principle component analysis for elliptical peak integration, and connected component analysis to identify and integrate arbitrary peak shapes.

Visualisation has become a fundamental part of the data-treatment, not just an end output. We have developed tools for showing, sorting and editing peaks lists overlaid on n-dimensional datasets. We have a number of harmonised tools to allow different perspectives on the same data, for example in three-dimensions of reciprocal space, via two-dimensional projections, and in detector space. We have used a range of third-party frameworks to achieve our visualisations ranging from VTK based ParaView3 to direct implementations in OpenGL depending upon our user-based visualisation needs.

**References**

[1] [www.mantidroject.org](http://www.mantidroject.org)

[2] O. Arnold, et al., Mantid—Data analysis and visualization package for neutron scattering and μSR experiments, Nuclear Instruments and Methods in Physics Research Section A, Volume 764, 11 November 2014, Pages 156-166, <http://dx.doi.org/10.1016/j.nima.2014.07.029>

[3] <http://www.paraview.org/>