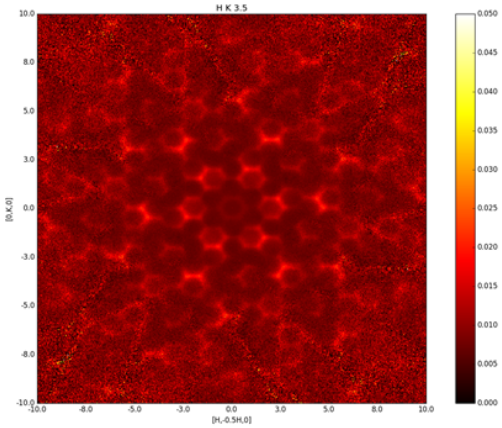
Data Handling for ESS Instruments Makes Headway in Collaboration With UK's STFC

AUG 07, 2017

ESS and ISIS. The ESS Instrument Data group at the Data Management and Software Centre is developing the Mantid Open Source Project together with STFC's ISIS Neutron and Muon Source in order to meet ESS instrument-specific requirements.

OXFORD and COPENHAGEN—The European Spallation Source (ESS) will be the most powerful spallation neutron source in the world, with a neutron brightness exceeding that of existing facilities by up to two orders of magnitude and producing a comparable increase in raw scientific data. The ESS Data Management and Software Centre (DMSC) in Copenhagen will be responsible for capturing that data and making it useful to the scientists running experiments in Lund. To do this, ESS is collaborating closely with existing neutron facilities to develop custom software based on the existing Mantid framework for data reduction.



An August 2017 visualisation of $LaNaF_4$as measured on the TOPAZ neutron instrument at the Spallation Neutron Source (SNS) in the US. Multiple orientations have been measured and stitched using Mantid software. IMAGE: Courtesy of SNS

Collaboration With ISIS Produces Results

Over the last 12 months the In-Kind Collaboration between ESS and the UK's Science and Technology Facilities Council (STFC) ISIS Neutron and Muon Source (ISIS) facility has made significant headway in improving the performance and flexibility of Mantid, bringing the project closer to meeting the unique requirements of the ESS instrument suite.

The team has also demonstrated that Mantid outputs can be connected to ESS live data streaming components. This is necessary for real-time data reduction, an important feature of the time-of-flight instruments at ESS.

Jonathan Taylor is the acting head of the DMSC and leads the data reduction work package at ESS: 'ESS and ISIS are collaborating on a range of projects that make up a high proportion of the scientific computing stack for ESS. For scientific computing, ISIS—as a world-leading pulsed neutron facility—is an essential partner for ESS."

Clockwise from top left: acting head of ESS DMSC Jon Taylor (r), in conversation with Ken Andersen, head of the ESS Neutron Instruments Divison, at ICNS '17 in South Korea (ESS); Owen Arnold at the NOBUGS 2016 conference hosted by DMSC; the ISIS data reduction in-kind team, including (l-r) Lamar Moore, Owen Arnold and Micheal Hart; Simon Heybrock of DMSC working on the Mantid instrument geometry code. PHOTOS: ESS and courtesy of STFC

Adapting A Common Framework to Exceptional Requirements

The ESS user programme will begin in 2023, when it is expected to produce 3-5 petabytes (PB) of data per year, rising to 7-11 PB over the following years. Aside from its high neutron flux and unparalleled instrument complexity, ESS will also require greater real-time capability for data reduction than has previously been attempted.

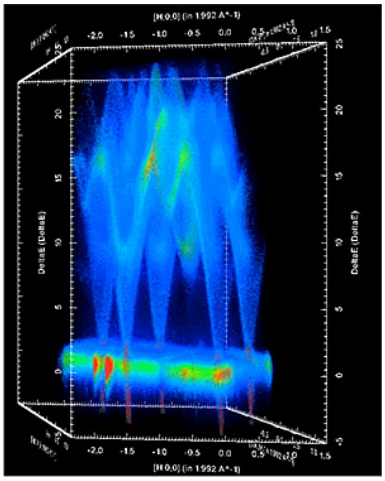
'The collaboration is really important," says Owen Arnold, who is leading the in-kind work package for STFC. 'We can call on experience from experts across different facilities for some of the hardest problems, and everyone benefits as we solve these forward-looking issues. The team at ISIS is very integrated with the ESS team, working on the same problems within the same code base."

The Mantid Project is an Open Source, neutron-specific data treatment framework. It was started by ISIS in 2007 to provide a common data reduction framework for all instruments at ISIS, and has grown into an international collaboration involving a large number of facilities. The inter-continental collaboration now includes ESS and ISIS, the Institute Laue-Langevin (ILL) in France, the Spallation Neutron Source (SNS) in the US, FRM II in Germany, and the Australian Centre for Neutron Scattering, ANSTO.

A Tide To Lift All Boats

Data reduction is the domain-specific term for a procedure that converts raw counts, as provided by instrument detectors, into scientifically useful data. At a basic level, this means accounting for geometry, efficiency and applying unit conversions. The reduced data can then be modelled into meaningful representations and returned to the instrument users as dynamic one-, two-, three- and four-dimensional visualisations of the particle interactions measured by the experiment. Exact workflows are dependent on the scientific technique, the instrument and the type of experiment.

The collaborative software development model maximises synergies across facilities and benefits from sharing the development workload and knowledge. This has been applied successfully in the past, for example, where SNS' expertise in event processing was adopted across the whole of Mantid.



Right: A Mantid visualisation of a non-orthogonal 3D projection of Spin Waves in Gadolinum as measured on the SEQUOIA neutron instrument at SNS. IMAGE: Mantidproject.org

'We also benefit where there is a requirement from another facility—for example, ILL's step-scanning instruments didn't really fit into the Mantid framework, and ILL was keen to roll Mantid out across its instrument suite," explains Arnold. 'Consequently the step-scanning element was accelerated to allow them to do this in a timely manner. For ESS, we can ensure things are done right using instruments at existing facilities way ahead of instrument construction at ESS."

An additional advantage to using a shared platform like Mantid is that it provides a familiar interface to neutron researchers as well as the scientists operating the instruments. Technique-specific functionality can be added to Mantid while maintaining a common look and feel.

'The Mantid project has shown the benefits of collaborative Open Source software development for large-scale facilities for many years," says Taylor. 'It is of great benefit to the ESS project as well as to the community of neutron users in Europe. The collaboration with ISIS will ensure that the ESS objective of delivering an integrated software suite for the instruments and user programme will be delivered, with the required functionality and

performance."

Mantid developers from ESS, ISIS and ILL at the UK's ACCU software conference earlier this year, from left: Martyn Gigg (ISIS), Owen Arnold (ISIS), Simon Heybrock (ESS), Lamar Moore (ISIS), Ian Bush (ILL), Matthew Jones (ISIS), Samuel Jackson (ISIS). PHOTO: Lamar Moore

###