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Dr Laurent Chapon
Head of Crystallography
ISIS

ISIS and Tessella Collaborate to Boost Scientific Output at World Leading Neutron Source

When ISIS received funding to build a second Target Station, they also saw the opportunity to invest in external professional software and project management expertise to help them develop an innovative new instrument-independent data analysis framework. The successful collaboration with Tessella will enable ISIS to provide its global scientific community with higher levels of overall user experience and service. The project has also been made available under open source licence for other neutron scattering facilities to use and extend.

Background

ISIS, located at the prestigious Rutherford Appleton Laboratory in the United Kingdom, is the world's leading pulsed neutron and muon source. The facility supports an international community of over 2000 scientists and has made a significant contribution to many of the major breakthroughs in materials science, physics and chemistry since it was commissioned in 1985.

The Requirement

In 2003 ISIS received funding from the UK's Science and Technology Facilities Council (STFC) to expand the center through the construction of a second target station designed to open up new opportunities in soft condensed matter, bio-molecular sciences,

advanced materials and nano-scale science.

This investment provided the ISIS team with the opportunity to explore a new approach to developing the software needed for the instruments and experiments that would be housed in the new target station.

Dr Laurent Chapon, Head of Crystallography and one of the main drivers behind the project explains "Software and data analysis tools are fundamental to our overall scientific process. They enable our community to generate and visualise the results of their experiments. This is particularly important for many of the new instruments in Target Station 2, some of which have hundreds of thousands of detectors and generate a volume of data similar to the Human Genome every day. However, until now it has been accepted practice within the science



community for software to be developed and managed by the scientists themselves, typically on an ad hoc instrument by instrument basis. There is a hidden cost with working this way - a lot of duplication of effort as well as poorly documented and tested code that scientists find it difficult to use and maintain."

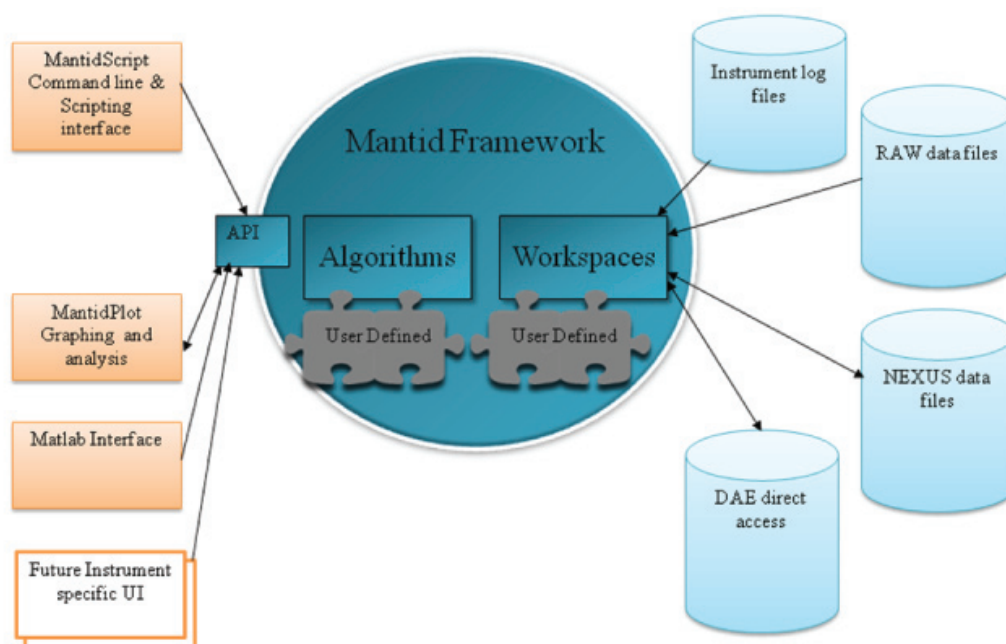
Prof Robert McGreevy, Head of Diffraction and Muon Division continues "We are investing significant sums of money into Target Station 2, and so it made perfect business sense to invest a small proportion of this in outside professional software expertise to help us create a reliable and extensible data analysis framework that would better serve our community of scientists. We also felt it was important to make the environment open source for other neutron scattering facilities to use and extend."

The Solution

A dedicated team was established staffed by full-time developers from both ISIS and Tessella. This not only creates close collaboration, but also a high degree of knowledge transfer

The team used a hybrid RAD (Rapid Application Development) approach to flesh out the initial framework, and then build out specific requirements using a monthly release schedule. This is not only an agile and flexible way of working, it also gives the scientific community the opportunity to shape the environment as it develops. To facilitate this Tessella run a Steering Committee made up of representatives from different scientific groups across ISIS.

The project is called Mantid (Manipulation and



A Unique Collaboration

ISIS tendered the project through Catalist, a UK Government list of approved suppliers.

"From the start we wanted the project to be a collaboration" says Prof McGreevy "and so it was important to find a partner that not only had a deep understanding of the world of science but also strong complementary expertise in project management, consultancy and software development. Tessella were a great fit. Their scientific experience meant they were able to very rapidly assimilate our requirements and translate them into reality."

Analysis for ISIS Data). As the name suggests, it provides an extensible data reduction and analysis framework for the ISIS neutron and muon data that is independent of instrument and analysis technique.

The framework can also be easily extended using a plug-in mechanism to add further user-defined algorithms, data structures and file formats.

Care has also been taken to isolate as much complexity as possible from the areas that may be extended by users, while providing them with powerful objects to manipulate their data.

The framework also provides a full virtual model of any instrument and its geometry using XML. This allows algorithms to be truly independent of the instruments, enabling complex attenuation



corrections and simplified diagnostics.

This could, in a later stage, greatly simplify the validation and use of simulated data, and allows simulated and real data to be compared and manipulated within the same framework. This will help boost scientific output and was something that was difficult to achieve in the past.

The Results

Mantid is now being rolled out to new instruments in Target Station 2 as well as replacing legacy software on instruments in the older Target Station. Scientists and project sponsors have been delighted with the ease of use and flexibility of the new environment.

Dr Chapon goes further “Aside from the software itself, I firmly believe that one of the major reasons for our success has been the expertise and professionalism that Tessella has brought to the project. They, of course, handle all the house-keeping tasks like release schedules, testing, documentation and code repositories, but more

scientists have usually booked their time months advance. Previously it might have taken days to resolve such an issue”

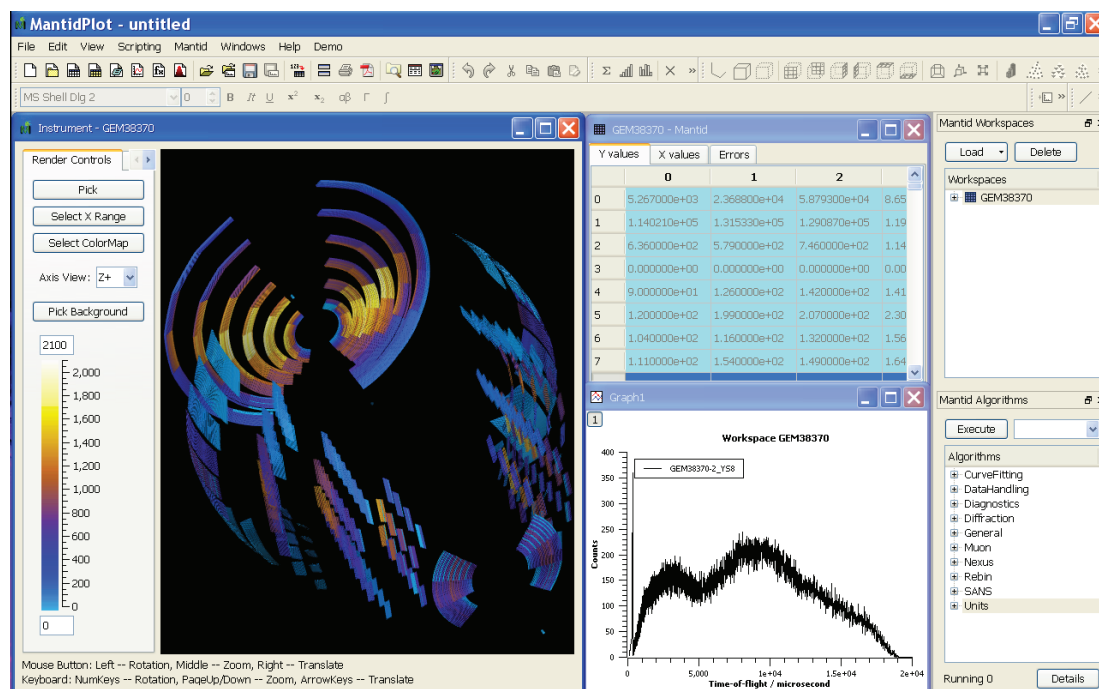
The team have also been able to redirect development resource to accelerate the urgent commissioning of new instruments.

“Investing in a professional, dedicated software team has resulted in significantly improved levels of user experience and service for the ISIS scientific community” says Prof McGreevy “which in turn helps us maintain our reputation as a world leading neutron source. Choosing to partner with Tessella is one of the best things we have ever done!”

The Future

The project team and Steering Committee will continue to use the monthly release cycle to shape the framework and applications.

As well as commissioning new instruments and upgrading legacy software on older instruments, the



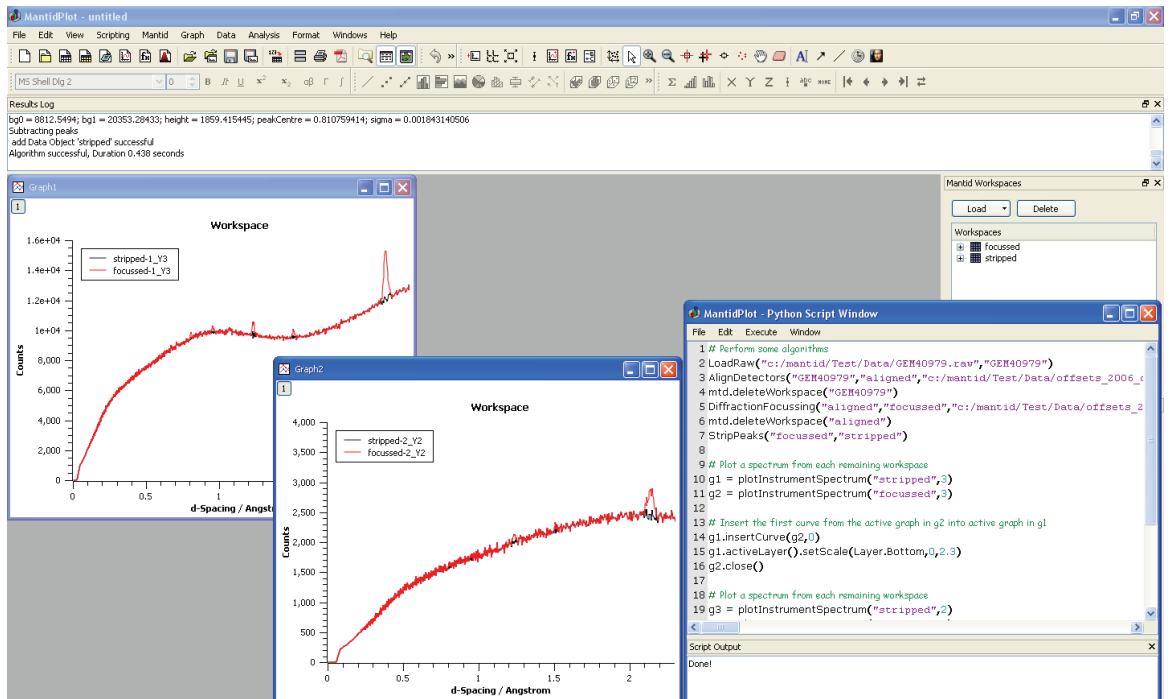
importantly are able to project manage and re-prioritise activity quickly in order to respond to urgent requests. In the last few months, prioritisation of the work has been crucial to enable the commissioning of new Target Station 2 instruments.”

For example, in one situation a scientist was unable to complete his experiment because of a software issue. “We logged the problem and a fix was produced within half an hour. This is significant when you consider it is costing tens of thousands of pounds a day to operate an instrument and

team are looking at ways of handling and visualising in very large multi-dimensional data sets, and integrating Monte-Carlo simulation techniques.

In addition, a number of neutron facilities around the world have expressed interest in adopting a similar approach to software development, as well as contributing to the framework.

The project output is released publicly at www.mantidproject.org under the GNU General Public License for use within the wider neutron community.



Scripting in Mantid

Requirements

- Easily extended instrument independent framework for data analysis
- A focus on the importance of software in the modern scientific process
- Professional, dedicated approach to software development
- Software & project management partner with background in science
- Project available to wider community as Open Source

Benefits

- Eliminates duplication of effort, and poorly documented and tested code
- Enables scientists to focus on the science rather than the software
- Increases productivity and scientific output
- Faster commissioning of new instruments
- Higher levels of user experience and service for the ISIS community
- Helps maintain ISIS reputation as world leading neutron source

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