ORNL Mantid Scientific Roadmap

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Software Development at SNS and HFIR

SNS and HFIR have changed their software development model in recent years. Software development is now a joint effort between the instrument staff, represented by a group of computational instrument scientists (CIS) and a group of software developers from ORNL's Computer Science and Mathematics Division. The recent focus has been on improving data reduction across the instrument suite. The SANS reduction software has been re-written in the past two years, and the reduction for diffraction and engineering diffraction will be completed by July 2021. Following that work, the engineering team will start working on new functionality across all instruments.

Mantid Usage at ORNL

ORNL joined the Mantid project in 2010. Since then, it has kept a significant level of resources focused on implementing the SNS and HFIR data reduction in Mantid, as well as contributing to the overall Mantid infrastructure. Although most of the development effort at ORNL was initially focused on Mantid, today's software landscape is more varied. In addition to remaining needs that are directly related to Mantid, a significant effort is directed towards user interfaces that use Mantid as a library. Data analysis software is also expected to become a focus area in the coming years.

Currently all neutron beamlines ORNL except imaging and triple-axis instruments are using Mantid as their reduction platform.

Recent Development Model Using Mantid

With the rewrite of the SANS reduction, the development of data reduction software to support SNS and HFIR has changed from a model where everything was implemented in Mantid to a hybrid model where Mantid is used as a dependency. A need was identified for a more lightweight and flexible implementation that instrument scientists can more easily read and use for more complex situations. In the case of SANS, a new dedicated python package called drt-sans (data reduction toolbox for SANS) was developed using Mantid for loading data and common algorithms. The new SANS software is executed as scripts, either directly or through a jupyter notebook.

Approaches to User Interfaces

Most instrument suites currently have working data reduction but are missing a dedicated user interface. The Mantid workbench provides a basic interface for several instruments (power diffraction, and certain spectroscopy beamlines). In some cases, standalone applications have also been developed (reflectometry, materials engineering). Jupyter notebooks is also being used (SANS, imaging).

Plans are being developed to create user interfaces built on a single platform to be shared by all instrument suites. This would allow a common look and feel across all instruments. Early design work is focused on developing a web application framework.

Status by Instrument Suite

The following is a very high-level view of where things stand according to the CIS group.

- **Diffraction**: The data reduction upgrade work is planned to be completed by July 1st. User interface work will be tackled along with other instrument suites.

- **Spectroscopy**: The most pressing need is for a new user interface. Analysis tools including resolution convolution are needed. The development of PACE at ISIS is of great interest.

- **Reflectometry**: Just like spectroscopy, the reduction is in good shape (changes can be made through maintenance work), but we are in need of a new and common UI. The existing reduction is only available through old unsupported versions of Mantid and python 2.7 applications.

- **Spin Echo**: There is an effort to design a UI for spin echo. This is in an early phase. The reduction itself is working.

- **Imaging**: Unlike the other techniques, there is no urgent UI work needed for imaging. There is, on the other hand, a long list of data processing needs. A lot of those items are dealt with by collaborating with external projects.

- **SANS**: SANS data reduction is generally in a good state. Current work includes integrating the use of an elastic scattering reference for EQ-SANS and general maintenance tasks. The USANS instrument scientist is investigating methods for data desmearing that he would like incorporated into the USANS data reduction.

- **Materials Engineering**: The VULCAN-X upgrade presently in progress on BL-7 will require effort to ensure the software is able to read, reduce, and analyze the data coming from the entirely new detectors on this beamline. The pyRS software for HIDRA still needs attention to address issues that were left out of the first release version.