ISIS Mantid Scientific Roadmap

Lamar Moore, Pascal Manuel and Toby Perring

May 2021

Introduction

This scientific roadmap outlines ISIS requirements and plans in relation to the Mantid software programme. This document represents the requirements of the science groups within the facility and will be presented on a technique-specific basis. However, this is informed by an over-arching strategy for scientific computing within ISIS. Any dates presented in this document are tentative and mostly flexible, however there are some time-bound milestones where we are required to deliver in order to maintain facility operations. ISIS remains open to suggestions on changes to the schedule to maximise collaboration with partner facilities.

Scope

This document contains the main scientific requirements which form our roadmap for Mantid projects. The technical roadmap which satisfies technical requirements for the project are handled separately. For completeness, the technical requirements are shown in the roadmap timeline at the end of this document. However, the scheduling and tracking of those requirements will be handled by the TWG in combination with the requirements below.

Muons

Wimda/MuSRFit -> Mantid

Critical functionality within the Wimda and MuSRFit packages are required for the running of the Muon science programme at ISIS. These are the DeFacto tools used by the Muon community and represent the gold standard for Muon analysis. There are major maintainability and usability issues with these packages looking ahead to the future which need to be addressed in the near term to avoid significant disruption or unsustainable workarounds. There has been a significant amount of effort thus far into subsuming key functional aspects of these packages. We are currently defining clear scope and resource requirements so that this effort can be delivered to our current time constraints.

Digitised Muons

Internal technological improvements to our data acquisition software on muon beamlines will imminently lead to a step-change in muon analysis capabilities. We need to investigate the impact on the Mantid platform as there will be an increase in data volumes and potentially the need for live processing of event-based Muon data.

Neutron Spectroscopy

General Requirements

There is a need for a better interface between Mantid and external third-party codes. This is largely being handled by the ISIS development team as part of a strategy for better dependency management. Further work will be required for better interfacing with ABINS, MDMC, MDANSE etc.

Neutron Compton Scattering (ISIS Vesuvio)

Currently implementing and updating algorithms within Mantid to improve performance and compatibility with more recent versions of the framework. Also planning for ETNA new instrument which will result in higher performance requirements. This largely impacts the fitting components of the framework which are on the technical roadmap for improvement.

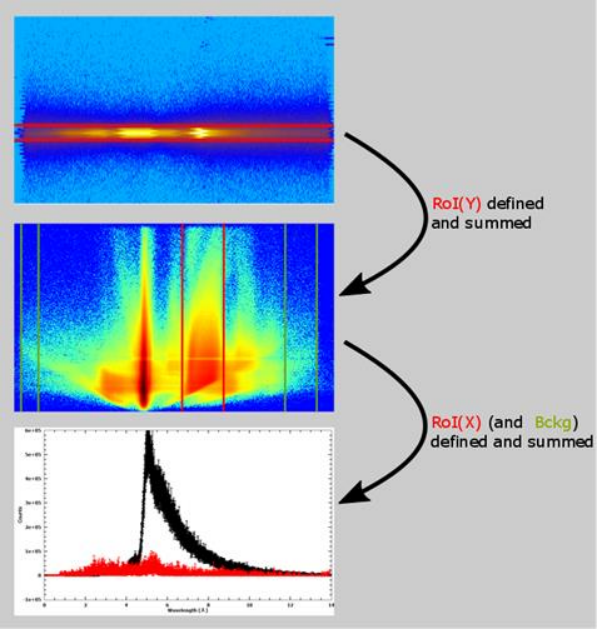
Neutron Reflectometry

2D Detectors

The NR group at ISIS has a requirement for a better approach to visualization and analysis of 2D detector data. Currently the functionality within the SliceViewer is only a subset of what is required for the group. Currently the definition of ROIs and associated integration of projections is not sophisticated enough to handle the SANS use case (described below).

Steps:

1. **Define RoI in one direction**
2. **Show integrated projection in Y and ToF**
3. **Define RoI and RoB (or a mask)**
4. **Show integrated projections of RoI and RoB if identified.**



"Complex" Beamline Geometry (Also Captured in Technical Roadmap)

The NR group requires more complex beamline geometry definitions within Mantid (and the associated IDF format). Currently Mantid assumes a direct path between sample and detector with very few exceptions. There is no concept of mirrors or guides within the framework to facilitate more complex L2 (or even L1) paths.

Small Angle Neutron Scattering

Processing Speed Improvements

Currently, processing in Mantid is a bottleneck in the SANS workflow as it is the slowest step (even slower than data acquisition). There are several items which need to be addressed:

- Parallelism of wavelength slicing.
- Parallelism for event (i.e. time) slicing.
- Improvement in file loading strategy as the SANS workflow is heavily I/O dependant.

Interface Configuration Improvements

The ISIS SANS interface is configuration is achieved using the TOML file format. This work is under way to improve the process of configuring the SANS reduction removing opportunities for error.

Spin-Echo (SE) SANS Reduction

The ISIS SANS interface currently performs the basic SANS reduction workflow. More work is needed to support the SESANS workflow.

Powder Diffraction

General Requirements

- Better calibration (including some feedback to instrument geometry and correct tracking of changes through the whole workflow)
- Improved ease of applying corrections (absorption, multiple scattering) that have been recently implemented.

Single Crystal Diffraction

General Requirements

There is a requirement to make Mantid more feature complete with respect to software for SXD in the Xray community.

- Proper and easy stitching of data from multiple angles for diffuse and Bragg scattering.
- More options for integration (especially for small peaks).
- Extinction corrections (needs interfacing to other programmes or implementation of Rietveld)
- User-friendly and meaningful data visualisation.
- Dealing properly with twinning/multiple crystallites by having an easy way to sort peaks is also a long-standing issue (which one to use for making one UB or separate satellite form main reflections etc) making multiple UB's and dealing with overlapping peaks either from different domain/twins for example. The rigidity of the workspace has been a blocker for this.

Neutron Imaging

General Requirements

Thus far, neutron imaging in ISIS has been focused on tomography and these requirements have been satisfied with the development of the Mantid Imaging platform which is used for pre-processing and performing tomographic reconstruction. Future requirements for imaging include:

- Energy-selective tomography.
- TOF Imaging.
- Integrating the NeXus Tomo Format into Mantid Imaging.

Disordered Materials

Gudrun/GudPy

A small percentage (≤10%) of the Gudrun codes have been absorbed into the Mantid framework for general use (mainly relating to total scattering and the generation of pair distribution functions). However, the core functionality of the software has not been entirely subsumed in Mantid. This is a large effort which will require a partnership between expert users of the software for scientific validation and target technical skills (extensive Fortran knowledge) if this will become a part of Mantid. To date, there is a short-term plan to create a python interface to Gudrun in the form of Gudrun which

will be overseen by ISIS. This has the potential of making Gudrun more accessible by other codes (including Mantid) but is not a suitable long-term strategy.

Timelines

Key: **Grey** – Technical Projects **Yellow** – Scientific Projects **Green** – BAU/Support **Red** – ISIS Shutdowns