Neutron imaging data processing using the Mantid framework

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Abstract. Several imaging instruments are currently being constructed at neutron sources around the world. The Mantid software project provides an extensible framework that supports high-performance computing for data manipulation, analysis and visualisation of scientific data. At ISIS, IMAT (Imaging and Materials Science & Engineering) will offer unique time-of-flight neutron imaging techniques which impose several software requirements to control the data reduction and analysis. Here we outline the extensions currently being added to Mantid to provide specific support for neutron imaging requirements.

1. Introduction
Several imaging instruments are currently being constructed at neutron sources around the world, including IMAT [1] at the ISIS facility, VENUS at the SNS and ODIN at the ESS. IMAT (Imaging and Materials Science & Engineering) is beginning its scientific commissioning phase in Autumn 2015. It offers unique time-of-flight diffraction techniques by capitalising on latest image reconstruction procedures and event mode data collection schemes which impose several software requirements to control the data reduction and analysis of its imaging data.

IMAT will provide neutron radiography (2D), neutron tomography (3D), energy-selective and energy-dispersive neutron imaging [1, 2]. Flexible neutron wavelength discrimination along this fourth imaging dimension via time-of-flight measurements is available at a pulsed-source facility like ISIS which opens up new opportunities for contrast-enhanced and microstructure imaging. For white-beam applications that do not need energy discrimination neutron counts in a wide energy band can be summed up to provide higher counting statistics. Standard data processing and reconstruction algorithms can be used for wide and narrow energy bands, with the limitation only being the reduced counting statistical errors for the latter. In this sense, energy-selective
neutron imaging is a straightforward extension of the two-dimensional radiography and three-
dimensional tomography methods. It is obvious that for best exploiting the information
content of such 4D data sets the use of high performance computer (HPC) clusters comes into
consideration, especially for time evolving experiments (5D) or on-the-fly image reconstructions
during data acquisitions. Furthermore, in addition to this direct imaging approach (wavelength
band selection), the transmission spectra of the imaging camera pixels may be analysed using
model-based fitting methods providing physical, elemental or structural parameters that can
then be reconstructed and displayed in two and three dimensions.

2. Frameworks

The Mantid software project [3, 4] provides an extensible framework that supports high-
performance computing for data manipulation, analysis and visualisation of scientific data [5].
The Mantid framework is mature and widely used across many facilities and techniques. It
is being extended to provide specific support for neutron imaging requirements. Being part
of the Mantid framework, the software introduced here effectively integrates with a vast array
of capabilities and methods readily available in Mantid. Mantid is open source, supported
on multiple platforms (Windows, Linux, Mac OS X), and packages are available for easy
deployment.

Here we introduce the imaging functionality that is being integrated in Mantid. A new custom
graphical user interface integrates reconstruction and visualisation capabilities for neutron
imaging. This interface (Figure 1) gives access to new features of Mantid to load images
and stacks of images into standard Mantid data structures and process imaging data. It
also provides access to third party software such as packages for tomography reconstruction
that support different 3D image reconstruction approaches for neutron tomography. Mantid
has the capability to run image reconstruction jobs either locally or in compute clusters and
supercomputing facilities thereby enabling quick evaluation and refinement of the reconstruction
pipeline.

Different facilities frequently choose different job scheduling tools and hardware for their
computing facilities. For example, the computer cluster SCARF (Scientific Computing
Application Resource for Facilities), which is available on-site for ISIS users, uses Platform Load
Sharing Facility (Platform LSF [6]). On the other hand the clusters at the Oak Ridge National
Laboratory and the SNS use the MOAB workload manager [7]. The Mantid framework provides
the middleware required to control jobs in different computing facilities handling the different
job schedulers and/or web service interfaces. The Mantid framework itself can be used through
its scripting interface via a web service API. This addresses challenges that arise at different
facilities, such as different authentication methods, job schedulers, and location of compute
resources.

Together with reconstruction functionality, Mantid also integrates multidimensional
visualisation tools that leverage on the VSI (Visualisation simple interface of the Mantid
project) [5], and the ParaView data analysis and visualisation application [8]. This provides
powerful tools to visualise the $\geq 4$ dimensional data that can result from imaging at a time of
flight spallation source (three spatial dimensions, wavelength, and conditions in time evolving
experiments). The VSI is a specialized application for neutron scattering data while ParaView
is a more generic application with which users can quickly build visualisations to analyze their
data, using quantitative and qualitative techniques. With both tools, the data can be explored
interactively in 3D visualisations, or programmatically via a command line interface, scripting,
and batch processing capabilities.
Figure 1. Mantid imaging interface integrated in the general Mantid graphical user interface with functionality for general manipulation and analysis of neutron data.

3. Compute resources at ISIS, STFC
Within ISIS, the SCARF and Emerald computer clusters, administered by the Scientific Computing Department at STFC (Science & Technology Facilities Council), will allow rapid refinements during the imaging experiments. A key hurdle is the ability to take full advantage of available computing resources. Different facilities frequently choose different job scheduling tools, interfaces and hardware for their computing resources.

At ISIS, users of the IMAT instrument will benefit from the high performance computing services provided by the ULTRA platform (Figure 2). This project, led by the Scientific Computing Department at STFC, aims at providing secure and efficient high performance computing and data services to support operations at ISIS and the Diamond Light Source.

The IMAT instrument requires advanced tomographic image reconstruction software that is able to deal with the energy dependencies in neutron imaging experiments. As a result, rapid 3D volume data reconstruction and in-experiment data rendering and visualisation with HPC based infrastructure are critical to IMAT experiments. In-experiment visual feedback to inform and guide experiments will optimise the use of beam time. Mantid is capable of using ULTRA2 high performance computing services in a way that is transparent to the user, via a standardised web service.

4. Tomography: reconstruction tools
The imaging interface being integrated in Mantid supports third party software for 3D image tomographic reconstruction. A number of tools are currently supported and/or being trialed: TomoPy [9], Astra Tomography Toolbox [10–12], and Octopus [13], and in the future the
reconstruction pipeline software Savu [14, 15] developed by the Diamond Light Source. Different reconstruction approaches are thus supported, namely filtered back projection and iterative methods such as simultaneous iterative reconstruction technique, but also variants of these developed in different tools.

5. Pre-/post-processing and visualisation

The new imaging features of Mantid are being tested with simulated and sample images. Mantid provides a harmonised and simple interface to different, heterogeneous tomographic reconstruction methods and tools which provide a varying degree of support for image pre-processing tasks.

Mantid is being extended with support for several input/output formats and additional parameterisation and pre-/post-processing functionality. This includes for example a graphical interface to select different areas, such as the region of interest for reconstruction, and the area for open beam normalisation (Figures 3 and 4). Support is being added for different data formats (FITS [17], NeXus NXtomo [16], TIFF [18], PNG [19], etc.) and variants of them. Additional capabilities are provided to process multi-dimensional stacks of images from energy-selective analyses, see Figure 5 for an illustration of the differences between energy neutron radiographies for different energy bands.

Image format extensions currently being defined for more specific processing of imaging data from IMAT also require integration in the framework. Different tomographic reconstruction tools support pre-processing and filtering tasks to a largely varying degree and in heterogeneous ways. Several pre-processing tasks that are essential for effective tomographic reconstruction are
Figure 3. Section of the imaging interface for interactive selection of different image parameters. The parameters, including center of rotation, region of interest, and open beam normalisation (or air region), are selected interactively in an interface that visualises a stack of images.

Figure 4. Section of the imaging interface where different pre-/post-processing filters and options can be defined. This includes for example enabling different types of normalization, detector specific corrections, and several pre-processing techniques for improving tomographic reconstruction results.
(a) Single energy band. (b) Average for a wide energy band.

Figure 5. Example images taken for testing purposes with the IMAT MCP detector, on a test beamline at ISIS.

Figure 6. Interface for the submission and control of remote reconstruction jobs. Multiple jobs can be submitted simultaneously, using common and specific parameters, and taking full advantage of the compute resources available on site for rapid in-experiment analysis and also off-site data analysis.

being integrated in a harmonised manner, considering different forms of image normalisation, filtering xand selection of regions of interest. All these components are integrated in a common graphical interface with which users can make an effective use of the tomographic reconstruction tools and HPC resources available (Figures 6 and 7).
Figure 7. Remote compute resource settings in the imaging interface of Mantid, including parameters, dataset selection, and user credentials for remote execution of reconstruction jobs on a HPC platform.

6. Future
Mantid and its imaging features are being actively developed. A custom graphical user interface, aiming at simplifying and harmonizing pre-processing and visualisation tasks, enables IMAT users to perform on-the-fly analysis of tomography data using high-performance computing resources. Long-term objectives include dealing with the multiple challenges posed by the complex datasets with three or more dimensions produced by energy-dependent tomography experiments: data volumes, better tailored pre-/post-processing, ease of analysis, etc. Equally important is aiding our users through the process of building their analysis workflows using the new features, and extending the tools on both the visualisation and manipulation and analysis sides as needed to support and optimise operations.

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