Tomographic reconstruction with Mantid Imaging

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Abstract. Mantid Imaging has been developed to provide a graphical reconstruction process for users of neutron imaging instruments to eliminate the need to fall back on commercial software. Mantid Imaging builds on algorithms provided by libraries including Astra Toolbox and Tomopy to offer noise reduction, artifact removal, alignment, filtered back projection and iterative reconstruction methods. Extra functionality was added by using algorithms from ALGOTOM for ring removal and from the Core Imaging Library (CIL) for regularised 3D reconstruction.

Mantid Imaging 2.4 has recently been released. It is an open source Python GUI, runs under Linux and Windows and can easily be installed on end user systems. Mantid Imaging is aimed at users with no programming background and with little image processing experience. At ISIS Mantid Imaging runs on the ISIS-Data-Analysis-as-a-Service (IDAaaS) platform, which is remotely accessible with any modern web browser and gives users access to sufficient hardware resources to handle large datasets. Extensions of Mantid Imaging for energy-resolved neutron imaging are planned for the future.

1. Introduction

Neutrons ability to penetrate dense solids and their sensitivity to nuclei make them a useful imaging probe for many materials studies. A neutron beam passed through an object produces a signal on a pixelated detector where the intensity of each pixel depends on the attenuation along the path. Neutron radiography and tomography find many applications in materials research and industry due to their potential for non-destructive testing and their ability for mapping low-Z elements, two main characteristics which make the neutron methods an effective and complementary probe to X-ray imaging.

A number of neutron images (or radiographs) can be recorded with the object rotated to different angles. From these the neutron attenuation within the 3D volume can be calculated for each voxel using tomographic reconstruction.

Neutron imaging is now being used in a wide range of fields including engineering, battery research, palaeontology, geology and cultural heritage. Neutron imaging is performed at a number of facilities including the ISIS spallation source in Oxfordshire, UK, on the IMAT [1], Engin-X [2] and INES [3] instruments. IMAT can image objects with a field of view of $200\,\text{mm} \times 200\,\text{mm}$ and with a resolution down to $60\,\mu\text{m}$. The instrument also offers Time-of-Flight (TOF) techniques such as Bragg-edge imaging, to map crystallographic properties of materials [4].

Mantid Imaging has been developed by the scientific software group at ISIS as an easy to use tool for neutron imaging users to pre-process and reconstruct their data, without requiring an in depth knowledge of the techniques involved. Figure 1 shows the main window with a dataset loaded. As the range of users from different research backgrounds grows an intuitive and well-designed graphical user interface

(GUI) becomes increasing important. Mantid Imaging takes care of specific processing requirements for neutron imaging and, after the termination of Octopus [5], supplements other open-source reconstruction packages such as MuhRec [6] and NeuTomPy [7].
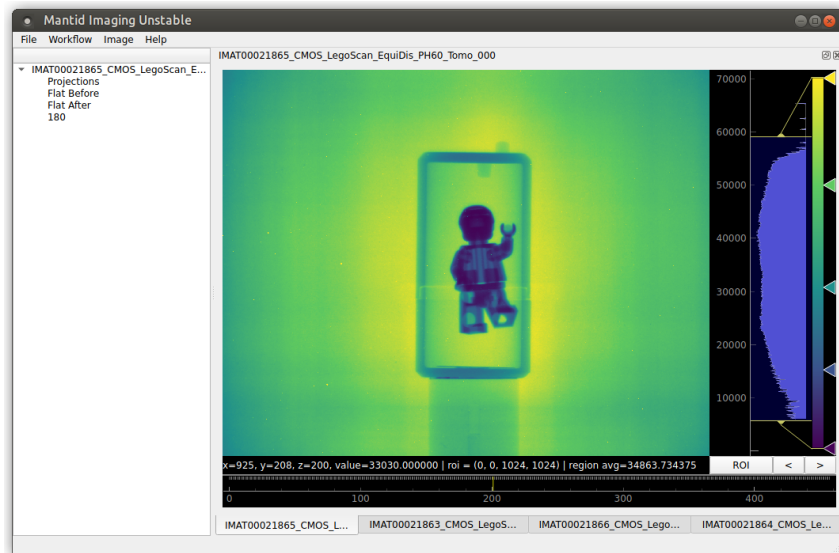
Figure 1. Main Mantid Imaging window.

Mantid Imaging [8] is free and open source, documentation and instructions for downloading and installing can be found at `https://mantidproject.github.io/mantidimaging/`.

2. Features
The features of Mantid Imaging are driven by the requirements of the IMAT instrument at ISIS to allow processing of neutron imaging data and tomographic reconstruction. The provision of pre- and post-processing operations in Mantid Imaging is essential for removal of image artifacts [9] and for obtaining meaningful reconstructed 3D datasets for further analysis.

2.1. Data handling
Neutron imaging experiments produce large 3 and 4 dimensional datasets. For the tomography use case, these are a series of 2D images (radiograms or projections) each with the sample rotated to a different angle. Here we consider rotation angle to be the third dimension. For other cases there can be a Time of Flight dimension to provide energy resolution instead of or in addition to the angle.

Most commonly, this data is stored in either a series of 2D TIFF or FITS image files or in a Nexus file by using the NXtomo definition. Nexus is based on the HDF5 format and supports multidimensional data arrays alongside rich metadata. Mantid Imaging can open and save datasets in any of these formats.

Typically, a dataset also contains flat field and dark images, which are used for normalisation. A flat field (or 'open beam') image is recorded with the sample removed, and a dark field image is recorded with the neutron beam switched off.

2.2. Pre- and post processing
Images acquired on a neutron imaging instrument require pre-processing before they can be input into a reconstruction algorithm. Mantid Imaging contains a collection of pre-processing operations that can be applied.

The signal recorded by the camera system is a neutron-intensity related quantity (e.g. photon count or charge) in each pixel. This must be converted to a transmission fraction. This is achieved using the flat-fielding tool which uses the dark and flat frames to subtract the background and normalise the images. Figure 2 shows a sample radiogram before and after such a correction. Conversion of transmission to attenuation is performed automatically at the reconstruction stage.
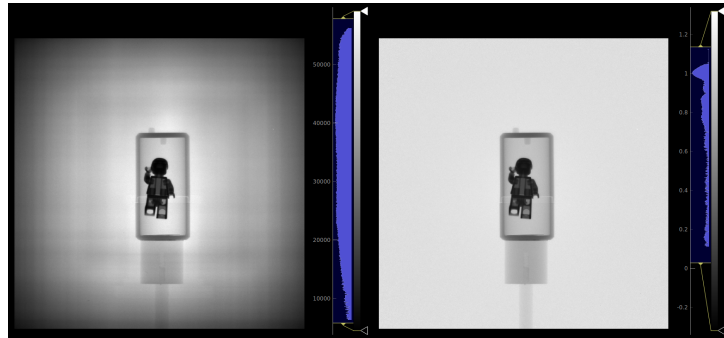
Figure 2. Sample projection before (left) and after (right) flat field correction.

Neutron images are prone to random and systematic errors, such as Poisson noise and collection-related artifacts due to instrumental misalignments or detector imperfections. Mantid Imaging has a choice of Outlier Removal (detected by difference from local median exceeding a user supplied threshold), Median and Gaussian filters that can be used depending on the data. There are also specific tools from Algotom [10] for removing stripe artifacts which would otherwise cause ring artefacts in the reconstructed slice. Mantid Imaging will convert the imaging data into sinogram space on the fly, as needed by the stripe filters.

There are also geometric filters to crop, rotate and resize images. Any of the operations can be applied before or after reconstruction.
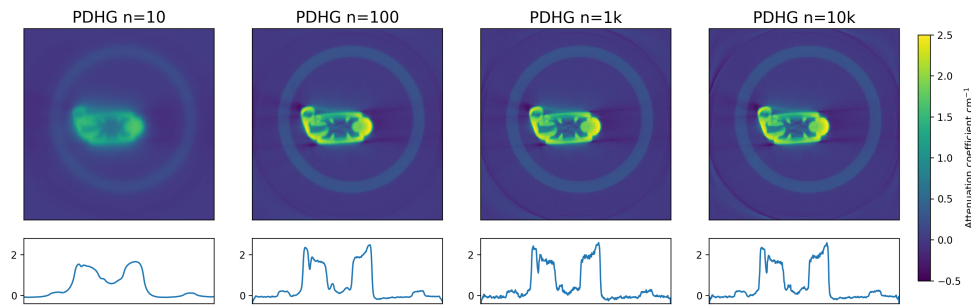
2.3. Reconstruction

The reconstruction stage takes the filtered and flat-fielded projection data and calculates the attenuation in each voxel in the volume. Mantid Imaging supports parallel beam geometry and offers correlation and iterative methods to align the centre-of-rotation and tilt. Mantid Imaging offers several algorithms for doing this as they each have specific advantages.

2.3.1. Filtered Back Projection Filtered Back Projection is a widely used technique for parallel beam reconstruction. Mantid Imaging makes use a GPU accelerated implementation from ASTRA Toolbox [11]. The user has a choice from several common reconstruction filters. FBP is fast and usually gives a good result, especially for fully completed 180 or 360 degree scans and for data with good counting statistics.

2.3.2. Simultaneous Iterative Reconstruction Technique (SIRT) Simultaneous Iterative Reconstruction Technique is an iterative technique that optimises towards a solution for the volume that results in the given projections. Mantid Imaging makes use of a GPU accelerated implementation from ASTRA Toolbox. The user has a choice of the number of iterations. SIRT can be more robust to noise, but the number of iterations must be chosen carefully to maximise detail.

2.3.3. Gridrec Gridrec is a Fourier grid reconstruction algorithm provided by Tomopy [12]. Gridrec is the only reconstruction algorithm in Mantid Imaging with a CPU implementation, so it can be used when a CUDA capable GPU is not available.

2.3.4. PDHG Primal Dual Hybrid Gradient is a regularised iterative algorithm for reconstruction, provided by CIL [13]. Mantid Imaging uses PDHG with an adjustable Total Variation (TV) regularisation term, α, and optionally a non-negativity constraint. TV is suited to samples with continuous areas of uniform material. Regularisation prevents over fitting to noise in the projections, preventing issues that can occur with simpler iterative algorithms. Increasing α pushes result to contain smoother regions. Figures 3 and 4 show the effect of adjusting PDHG parameters.

Figure 3. Slice and central line profile from a PDHG reconstruction with varying number of iterations, *n*, from 10 to 10,000.
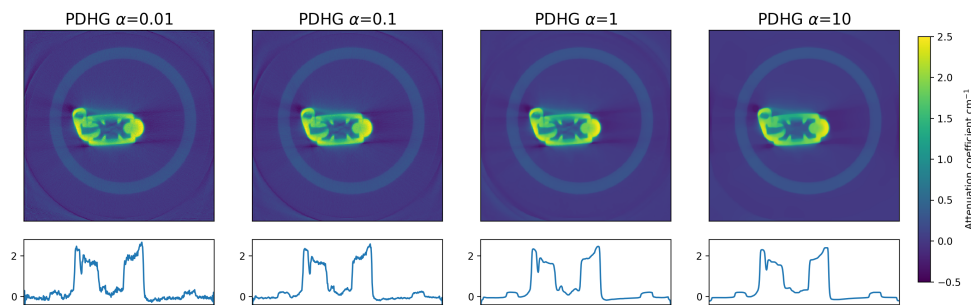
**Figure 4.** Slice from a PDHG reconstruction with varying regularisation parameter α from 0.01 to 10.

3. User interface

The user interface is divided into three windows, a main window for loading and viewing datasets, an operations window with pre and post-processing tools and a reconstruction window. There are also dialog windows for loading, saving, viewing metadata operations and other activities.

Mantid Imaging is built on the principal of being quick and easy to explore the data, and to visualize the effects of filters and operations. The windows provide a consistent 'image view' widget that allows zooming and panning, scrolling through the 3rd axis and control of the displayed brightness and contrast.

The main window features a side panel with treeview of the loaded datasets and a tab image stack viewer. It can be used to explore the data, for example to check for quality and artefacts. It provides tools for loading and saving data.

The operations window uses a 3-panel view to show a before and after view of the filter being applied as well as the pixel difference between them. Figure 5 shows an example with the remove outliers filter. The reconstruction window shows projection, sinograms and a preview of a reconstructed slice.
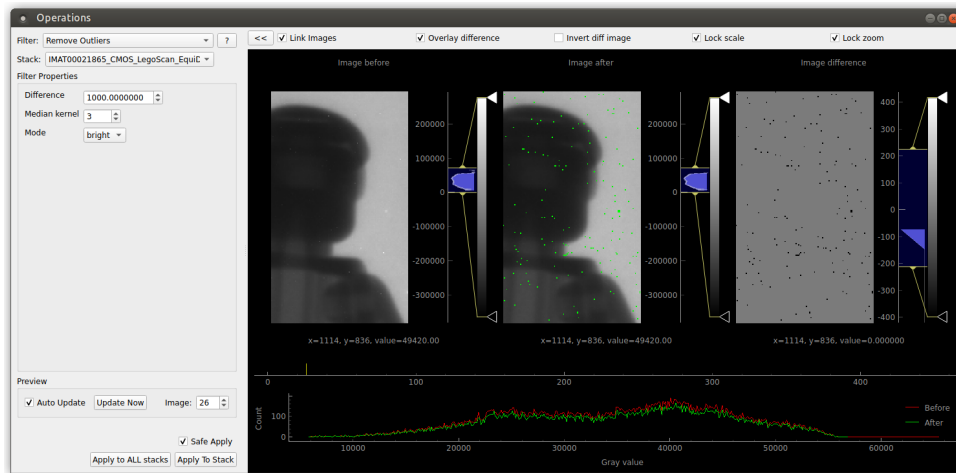
Figure 5. Operations window showing the remove outliers filter.

4. Development

4.1. History

Mantid Imaging was originally created as tool for handling neutron imaging data within the larger Mantid software project [14, 15, 16] in 2016. Its development was driven by the construction of the IMAT imaging beamline at ISIS which came online in the same year. After initial prototyping work and due to differences in imaging and neutron scattering data structures, Mantid Imaging was split into a separate software project with its own independent code-base. The GUI was created in Python, using PyQt and PyQtGraph to allow rapid development.

For the initial phase of IMAT operation, the commercial reconstruction package Octopus [5] was used for the majority of experiments. When the Octopus publishers announced that they would stop supporting the package, Mantid Imaging was prioritised as a replacement. With the first end user release, 2.0, in January 2021, it supported standard workflows and allowed IMAT to begin to transition. Further releases followed, through to 2.4, expanding the capabilities of Mantid Imaging and improving the user experience. It is now the main tool used at IMAT for white beam imaging and reconstruction.

4.2. Methodology

Mantid Imaging has been developed by the data reduction team in ISIS scientific software group. We use scrum agile methodology adjusted to suit the small size of the team. By having frequent meetings between the developers and the IMAT instrument scientists features can be prioritised based on research needs.

We use Git for revision control, hosted on GitHub. The service also provides issue tracking and automated testing, allowing a suite of unit, system and graphical tests to be run on each pull request before merging into the main branch. Nightly builds are automatically made available and installed on IDAaaS for manual testing. Stable release are made several times per year.

Mantid Imaging makes use of 3rd party libraries to provide features and speed development. For data handling, imaging loading and simple operations Mantid Imaging uses common scientific python libraries: Numpy, Scipy, tifffile, h5py, astropy and scikit-image; as well as some more specialised libraries: Tomopy [12], Algotom [10], Astra-toolbox [11] and the Core Imaging Library [13]. These dependencies are managed with Conda.

5. Outlook

Mantid Imaging is under active development to improve usability, performance and increase its versatility: The current focus is support for golden ratio scan datasets and cases with missing angles; Integration of newer reconstruction methods from CIL to better handle these data sets; Simpler installation on Windows computers. There is also a project to enable handling of Time of Flight datasets.

Acknowledgements

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