Mantid (and data reduction) at ILL: Scientific roadmap (May 2021)

Current situation and resources

The implementation of Mantid at ILL is taking place as part of the Endurance modernization program (within the Bastille project to improve the analysis software).

During the first phase of the project (March 2016 – March 2019) three software developers worked under the lead of a Tessella expert (during the first two years) to implement Mantid for time-of-flight (direct and indirect geometry), powder diffraction, small angle neutron scattering and reflectometry.

The second phase of Bastille started on December 2019 and will extend until April 2023. The available human resources during this phase are three software developers (with 3-years contracts) that work under the lead of Gagik Vardanyan (permanent staff at the scientific computing group). The main goals consist in consolidating the work done during phase I and extending it to a suite of instruments that were not included in that phase. Our objective is that by 2023 Mantid becomes the reference analysis framework for approximately 20 instruments at the ILL.

Beyond 2023, the effort and resources that will be dedicated by the ILL to ensure the maintenance and further developments of Mantid are still to be defined.

At present, Mantid has become the main data reduction software for half a dozen instruments. In some cases (new or upgraded instruments), it is the only available tool to read and treat the raw data. For other instruments (in particular powder neutron diffractometers, reflectometers and some SANS machines), we are in a transition period and old software (e.g. Lamp, Grasp, etc.) and Mantid live together, with users choosing one or another depending on their own experience and preferences. However, we expect that after the long ILL shutdown (October 2021 to ~December 2022), Mantid will become the main framework to perform the data treatment at ILL. In particular, Lamp will be frozen and maintained only to allow reading and reducing old data, but without any active support from the scientific computing group.

Data reduction at ILL by technique

1. Time-of-Flight direct geometry spectrometers

Instruments: IN5, Panther and IN6-Sharp (CRG).

Mantid is in use and the situation can be globally considered as satisfactory, with Mantid being able to handle the data reduction for all the relevant use cases.

For single crystal work, Mantid is used to read, pre-treat, and produce the input files needed by Horace, which is the analysis software preferred by most of our users for this kind of work.

2. Backscattering (and time-of-flight indirect geometry) spectrometers

Instruments: IN16B and IN16B-BATS. IN13+ (CRG) in 2023.

Mantid is in use in IN16B (standard backscattering spectrometer, with the incident energy defined by a monochromator mounted in a Doppler machine), including the handling of the diffraction detectors and the BATS mode (incident energy defined by TOF of a chopper generated pulse), and the situation is judged as satisfactory.

IN13+ will be an upgrade of the current IN13 (a thermal backscattering spectrometer) that will benefit from the new H24 guide. When the new instrument will be commissioned, the existing algorithms developed for the other spectrometers will be simply adapted to it.

3. Powder neutron diffraction

Instruments: D20, D2B and D1B (CRG). XtremeD (CRG) in 2023.

Mantid can be used at the ILL powder diffractometers and manages correctly the scan-like acquisitions used in D2B and occasionally in D20. Particular tools need probably still to be developed to facilitate and automatize a few tasks required for some experiments, but this work has to be done in collaboration with the instrument scientists and will likely involve only the development of specific scripts.

XtremeD is a new diffractometer for extreme conditions under construction now. We foresee to apply directly the same algorithms and workflows already in use in D20 and D1B.

4. Single crystal monochromatic neutron diffraction

Instruments: D3 (polarized neutrons), D9, D10, D19, and D23 (CRG).

Not foreseen in Mantid (not included in Bastille’s project) and not a priority for concerned scientists, which are using other tools (e.g. Int3D).

However, following recent discussions with ISIS and SNS about the developments going on there in this field, we are ready to collaborate with other facilities to explore the potential of Mantid for single crystal diffraction.

5. Single crystal Laue neutron diffraction

Instruments: CYCLOPS, OrientExpress, and LADI+DALI (Quasi-Laue for protein crystallography).

Not foreseen in Mantid (not included in Bastille's project) and not a priority for concerned scientists, which are using other tools (e.g. Esmeralda and LaueGen).

6. Diffuse scattering diffraction (and spectroscopy)

Instruments: D7 (polarized neutrons).

D7 is a general purpose spectrometer with full neutron polarization analysis capability. It is mainly used to study magnetic short-range order, but also to separate coherent/incoherent contributions to the static structure factor and occasionally as a TOF spectrometer to separate collective and single particle excitations.

Work to be able to use Mantid to reduce D7 data has been completed recently for the powder diffraction case. Additional developments to handle single crystal and TOF measurements are ongoing and should be completed during 2021.

7. Disordered materials diffraction

Instruments: D4 and D3-liquids (polarized neutrons).

Similar instruments are SANDALS and NIMROD at ISIS and NOMAD at SNS.

At present both instruments use their own suite of routines written by the instrument scientists to perform the data reduction. For D4, the use of a python notebook as an alternative for the data reduction has also been demonstrated recently.

Data reduction workflows will be implemented in Mantid for D4 and D3-liquids during 2021-22. Both are scanning instruments (detectors have to be moved and several acquisitions performed to cover the whole angular range), so the same solutions already applied to D2B and D20 will be used here. Most of the correction steps are standard (e.g. background subtraction including attenuation coefficients and vanadium normalization to obtain the differential scattering cross section in absolute units), but in addition algorithms to perform inelasticity (Placzek) corrections and Fourier transform the static structure factor to produce distribution functions in real space will be needed.

8. Strain imager for engineering applications.

Instruments: SALSA.

The instrument loader and corresponding reduction workflow will be implemented during 2021-22. We foresee to use similar algorithms and scripts to those already used for powder diffraction.

In parallel, instrument scientists are also interested in the possibility of using STeCa (Stress Tensor Calculator), a software used at FRM-II. While STeCa is a tool oriented to the data analysis, it can also be used for the data reduction part, so this could be an alternative to Mantid.

9. Small angle neutron scattering.

Instruments: D11, D22, and D33. SAM (CRG) in 2023.

Mantid can be used in the ILL SANS instruments since the first cycle of 2021. There is still some fine-tuning going on and efforts to make it more efficient and user-friendly when dealing with large data sets, but the standard cases (isotropic scattering, integration by sectors, 2D reduced data) can already be treated now.

One of the possible improvements under discussion is a more detailed calculation of the instrument resolution, using numerical convolutions and/or a ray tracing approach ("à la Grasp") of the different elements that define the Q-resolution.

General improvements in the plotting tools (see below) should provide a more friendly way of visualizing and manipulating large sets of data.

We also need to consider if all the functionality existing in Grasp to work with 2D data (in particular related to crystalline and/or magnetic samples) is available or should be made available in Mantid. Some of the tools provided by Grasp are very specific or at the frontier between data reduction and data analysis, so this is still an open question.

Finally, complementary simultaneous measurements can be now performed in all these instruments, e.g. SAXS+SANS in D22, DLS+SANS in D11, UV+SANS, etc. At present, such acquisitions are managed by a separate equipment and hence treated in an independent way. However, in the future Nomad (our instrument control software) should control also such complementary equipment and their data will be registered in the same NeXus file as the neutron data. Hence, we could need to extend Mantid to load and manipulate such "non-neutron" data.

SAM will be an standard SANS D11-like instrument, so no new developments will be needed.

10. Time-of-Flight reflectometry

Instruments: D17 and Figaro.

The work to implement Mantid for D17 (in TOF mode) and Figaro has been completed. The data reduction workflow will be tested and improved during the two reactor cycles in 2021.

We still need to find a good solution to correct for gravity effects, which in some configurations are particularly relevant.

11. Monochromatic reflectometry

Instruments: D17 and SuperADAM (CRG).

No immediate developments foreseen. SuperADAM scientists use and maintain their own software. Discussions about the D17 case should start once the TOF mode is fully tested.

12. Small momentum transfer diffractometer

Instruments: D16.

D16 is a multipurpose instrument with applications in a large number of fields. It can operate as a SANS/WANS instrument, covering the gap between the standard SANS machines and D20 or D4, as well as a reflectometer.

Implementation of Mantid at D16 has started and a few diffraction experiments have already been treated using Mantid. This work will continue during 2021, ensuring that Mantid can cover all the needs demanded by the different operation modes available in D16.

13. Neutron spectroscopy

Instruments: Lagrange.

Similar instrument to TOSCA at ISIS and VISION at SNS.

Mantid will be implemented for Lagrange during 2021. From the geometrical instrument definition this is a quite simple case, so no special developments or difficulties are expected.

Nowadays, parallel DFT calculations are frequently needed to interpret the neutron spectra, so Lagrange will benefit of the work already done in Abins and future developments there.

14. Neutron imaging and tomography

Instruments: NeXT.

Implementation not foreseen in the current phase of Bastille. However, this is a new instrument being commissioned now and we still need to discuss possible solutions concerning data treatment here.

15. Neutron spin-echo

Instruments: IN15 and WASP.

No plans at present. Data reduction software developed and maintained by instrument scientists.

16. Triple axis spectrometers

Instruments: IN3, IN8, ThALES, IN20, IN12 (CRG), IN22 (CRG).

No plans at present. Data reduction software developed and maintained by instrument scientists.

17. Nuclear and Particle Physics

Instruments: FIPPS, PF1B, PF2, PN1, PN3-GAMS, GRANIT, S18 (CRG).

No plans at present. Data reduction software developed and maintained by instrument scientists.

General developments and interests

1. Common "spread-sheet" like user interface

A new interface (DrILL) has been developed to respond to the requests of SANS and reflectometry scientists. We plan to extend it to all ILL instruments, allowing treating efficiently standard experiments where the same reduction procedure has to be applied to a large number of samples.

2. Overplotting ("Superplot") tool

Plotting tool designed to facilitate the comparison and the exploration of Mantid workspaces, e.g. scrolling through equivalent cuts (horizontal or vertical) in selected workspaces. A first version is already available.

3. Raw data explorer

Another plotting tool to facilitate and accelerate the visualization of raw data during the experiment. The idea is that a series of simple Mantid commands (e.g. load a data set, apply an algorithm to transform the raw data into something meaningful to the user, e.g. I(Q), and then plot it) is replaced by a single click on a button in an interface. This will require some work to embed the instrument viewer in such interface.

4. Event mode data

While not heavily used until now, acquiring data in event mode is possible in most of the ILL instruments and this can be very useful for some kind of experiments. A converter to rewrite the raw binary event mode data registered by the ILL electronic cards into Event NeXus files has been already written, in order to use Mantid capabilities to handle the event mode data. However, there are some specificities related to the link of the original design of the Event NeXus format to spallation sources that need to be understood or improved before we can use this format to manipulate and filter our event mode data. We are currently working on this.

5. Multiple scattering corrections

Many users would like to have access to a modern version, but easier to use if possible, of the traditional programs to evaluate and correct multiple scattering (e.g. MSCAT, Discus, etc.). While there are some algorithms available in Mantid[1], we need to check if they provide all the functionality demanded and can be applied and used directly in all our reduction workflows.

6. Data analysis in Mantid

The indirect data analysis interface is occasionally employed by some users, but our policy is that Mantid should be essentially a data reduction framework and that the complexity and variety of possible data analysis procedures are better handled outside Mantid.

7. Automatic (live) data reduction

Nomad can launch standard data reduction auto-process algorithms by communicating with Mantid via Cameo. We plan to use this approach to perform automatic data reduction during an experiment without requiring any human action. This will facilitate that users can take quick decisions based on treated data instead of relying on the raw data or waiting until a manual data treatment is performed. Reduced data could also be used to automatically program some data control decisions, such as stopping an acquisition when the statistical quality of the acquired data is good enough.

This requires a parallel effort in the acquisition control side, which includes a well-defined acquisition strategy and a correct tagging of the samples. This work is currently being done by the SCI group. Recently a collaboration between the ILL and Berkeley (gpCAM) has also demonstrated the use of Artificial Intelligence to pilot the data acquisition, so in a longer term we could envisage fully automatic acquisition+reduction workflows.

[1] https://docs.mantidproject.org/nightly/concepts/AbsorptionAndMultipleScattering.html