***Mantid - the next 5 years***

Mantid is the focus of a software collaboration between large scale facilities which is unique in the N, X and other fields. It

* is a sophisticated, state-of-the-art code which is developed in a highly professional manner across two major facilities.
* currently serves ~40 instruments to differing extents at ISIS and SNS.
* provides transparency and accountability which is rarely seen in scientific software development.
* removes single points of failure and individualism that have plagued software development.

Context

Can't look forwards 5 years without looking back over the first 10 years.

ESS and ILL joining the project.

ILL is operational and needs to replace LAMP for ~20 instruments as quickly as possible - next 3 years.

ESS will have first neutrons in 5 years, first users in ~8 years.

Mantid and the consortium/collaboration (NSSC)

Mantid is the name of a software project mainly for data reduction.

Mantid is the focus of a neutron science software consortium/collaboration (NSSC) which can develop and/or drive more than data reduction i.e. data analysis, modelling, data management (catalogues/databases/etc) and software infrastructure (PC, workstation, clusters, HPC, cloud/stack, etc).

Analysis software should be collectively developed and maintained to cover the majority of neutron scattering techniques (especially high throughput): diffraction - GSAS (SNS?), FullProf (ILL), SANS - SasView\* (ESS), reflectometry\* (FRM2), imaging\* (PSI), QENS\* (ILL), INS\* (ISIS), magnetic excitations. \* indicates software to be developed and supported in the SINE2020 EU project, which includes PSI and FRM2, as well as ISIS, ESS and ILL – the named facility is the developer on behalf of the consortium.

Modelling in this context is mainly molecular dynamics (MD) and lattice dynamics which are both provided by a wide range of classical and DFT simulation codes. The output from these simulation types and codes needs to be coupled to neutron scattering experiments e.g. nMoldyn (to be renamed MDANSE) for MD, supported by ILL.

McStas may also be regarded as a modelling code to be integrated in data reduction/analysis, supported by DTU/ESS/ILL(?)

The first 10 years

Mantid was originally designed for static, time-of-flight, spallation source instruments (at ISIS). This design legacy probably hinders adpating Mantid easily to a wide range of instruments e.g. geometry for scanning instruments at reactor sources.

The pressure to deliver functionality, starting from zero, has probably led to some case-by-case solutions which need rationalising.

The initial design legacy and 10 years of continuous development probably lead to a significant level of technical debt which should be reduced before the next phase of development.

Mantid was initially a C++ framework which has acquired a rich, Python interaction layer which is still not regarded by some as being easy enough to use.

What is Mantid

Mantid = Framework + algorithms + visualisation + interface (+ fitting)

Mantid is a data reduction framework and algorithms for data reduction for all instruments and techniques

Mantid may provide data analysis where external codes are not clearly identified (e.g. QENS) or where there has been a clear decision to integrate analysis (e.g. Horace -> VATES for INS)

Mantid must provide data visualisation for neutron scattering data, especially multi-dimensional data (e.g. VATES/VSI, sliceviewer, etc)

Publication quality plotting should be available where reasonably possible and exporting data to widely used plotting software must be easy.

MantidPlot is a generic interface to Mantid which is well-adapted for 'expert/instrument scientist' use.

Simpler interaction with Mantid is required for straightforward measurements and non-expert users. Very simple, web-based user interfaces, that are also the basis for auto-reduction, are probably best-suited, given that future data treatment will probably be cloud-based. Data visualisation tools are still required in this case.

The next 5 years

The scope of Mantid needs to be carefully defined and limited. In the spirit of a neutron scattering toolbox, data reduction is inherently limited by the instruments, techniques and science and there is not much new in this respect. Development should plateau to a certain extent. New requirements will come from new instruments (ILL and ESS), higher data rates, new IT infratsructure, etc.

Limit the number of levels of interaction with Mantid, currently C++, Python, MantidPlot, UI’s, web UI’s, auto-reduction. (I recollect that Mantid started as mainly a C++ code on the basis that scientists would not develop code. The Python layer has evolved considerably to enhance this but we are now aiming to cater for an increasingly large fraction of non-expert users and provide auto-reduction so the Python layer could possibly disappear in the future.)

Avoid risk of endless programming effort to cover all user requests (especially plotting and interfaces) – at some point users have to adapt to the software (as with existing, crappy, antiquated software!) and one piece of software cannot adapt to all the requests of the very large Mantid user base.

Very high level of functionality already exists in Mantid. Delivery of new functionality could be slowed down and significant effort spent (if necessary) on cleaning and refactoring, removing redundancy, reducing technical debt, limiting impact of legacy, facilitating software development in C++ and Python, etc. Independently audit the code/project to determine the effort to be spent on this.

Deliver key scientific components for e.g. self-shielding, multiple scattering, multi-phonon contributions.

Ensure that final adaptation of existing work is made in key areas so that Mantid can be accepted by users e.g. sliceviewer <> Mslice

At ILL, implement ~20 instruments in Mantid and deploy. Pragmatic approach with respect to users has to be adopted to deliver the software in the time frame (3 years). A cleaner implementation can be envisaged if necessary in the medium term.

Vision

At the end of the next 5 year period, data reduction should (largely) disappear from the scientist’s workflow. Instruments should systematically produce reduced data.

Effort supporting data reduction should stabilise at a lower level and the consortium (NSSC) should be able to commit significantly more effort to data analysis.

Data analysis and modelling software should be seamlessly integrated with data acquisition and reduction. Scientific results should be produced during experiments, guiding decisions during experiments and optimising use of beam time.