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Report to ISIS Mantid PMC
26 January 2015

Report on the usage of Mantid at ISIS

Remit

- To gather current Mantid take-up and usage information across ISIS science activities.
- To assess whether the move to Mantid has accelerated or retarded science output at ISIS.
- To gather short-, mid- and long-term requirements from ISIS science groups and identify areas of current underperformance which need to be urgently addressed.
- To identify common themes across ISIS science groups in order to inform the ISIS Computing Strategy and re-evaluate the Mantid project aims and milestones.
- To assess the current model of interaction between ISIS scientists and the Mantid group.

Executive Summary

- Mantid is commonly praised for it's open source and cross-platform approach.
- Interactions with SNS are proving useful and helpful amongst Mantid users.
- The usage of Mantid varies significantly across different science areas in ISIS
- The interaction of the science groups with the Mantid team is patchy.
- The visibility of the Mantid group within ISIS and externally is low (communication). e.g. no links to Mantid from ISIS computing pages. Poor knowledge of Mantid Group activities. Lack of scrutiny over scientific priorities.
- Scientific priorities are set piecemeal on a group-by-group basis.
- Some science areas - notably QENS,DINS and Mol Spec, Muon Spectroscopy, Powder Neutron Spectroscopy, Reflectometry and SANS are "heavy users" of Mantid. Generally their interactions with the Mantid team are good.
- Some areas make extensive use of Mantid, in conjunction with other software packages either locally produced or proprietary. i.e. Single Crystal Spectroscopy and Powder / Single Crystal Diffraction.

- There are two science activities that currently don't make any use of Mantid - namely, Disordered Materials Diffraction and Engineering / Imaging. Disordered Materials Diffraction does not plan to used Mantid in the next 5-10 years. Engineering and Imaging have a strong desire to use Mantid.

- There are some common scientific requirements coming between science activities to do with

    - **Speed** (loading files) (Reflectometry, SANS, Single Crystal, Spectroscopy, Muons, Powder diffraction)
    - **Lack of absorption and multiple scattering corrections** (Powder diffraction, single crystal diffraction, SANS, Disordered Materials, Spectroscopy)
    - **Lack of multi-dimensional data visualisation and reduction usability** (VATES) (Single Crystal Spectroscopy, Single Crystal Diffraction, Reflectometry)
    - **Fragility of reduction routines on release of new versions of Mantid** (Muons, Powder Diffraction, Spectroscopy, MoI Spec and QENS)
    - **Low quality graphics** (Reflectometry, Muons, Spectroscopy)

- There is much less agreement between groups on:

    - GUI vs. script interfacing
    - Modelling within Mantid vs. interface to external modelling code (i.e. "where does Mantid stop")
    - Whether harmonised approach across instruments is necessary / desirable.

Science group input

The survey is built on meetings held with ISIS science groups between the 6th and 15th January 2015. These groups do not follow the ISIS instrument groups is all cases.

The science groups were asked to explain how they currently use Mantid on their instruments. There were various levels of usage of Mantid identified:

- Data Inspection (e.g. instrument view)
- Live Data
- Instrumental Calibration (e.g. positions, distances of detectors, PSD calibration, etc.)
- Data Correction (e.g. background subtraction, vanadium normalisation, etc.)
- Data Reduction (e.g. coordinate conversion, Q-space rebinning, cutting, etc.)
- Fitting
- Modelling (e.g. ab-initio calculations, Monte-Carlo, etc.)
- Log Book
- Publication quality figure production

Each group was additionally asked to discuss the advantages and disadvantages of using Mantid on their instruments, by comparison to other (current or legacy) software used. The groups were asked to assess their current interactions with the Mantid team with regard to the responsiveness of the Mantid group to their running requirements. Additionally, they

were asked about interactions with their counterpart science groups at the SNS and elsewhere.

The future requirements of each science group were discussed, these being generally based on user and instrument scientist input.

Science group	Participants
Reflectometry	Tim Charlton John Webster
Small-angle Scattering	Steve King John Webster
Single Crystal Diffraction	Pascal Manuel Matthias Gutmann Steve Hull
Single Crystal Spectroscopy	Helen Walker Rob Bewley
Powder and Disordered Materials Spectroscopy	Ross Stewart
Disordered Materials Diffraction	Sam Callear Daniel Bowron
Quasi-elastic scattering, Deep Inelastic Scattering and Molecular Spectroscopy	Sanghamitra Mukhophadyay Svemir Rudic Franz Demmel Felix Fernandez Alonso
Powder Diffraction	Aziz Daoud-Aladine Matt Tucker Craig Bull Steve Hull
Engineering and Imaging	Winfried Kockelmann Shu Yan Zhang Joe Kelleher Saurabh Kabra
Muon Spectroscopy	Steve Cottrell Adrian Hillier
Training	Helen Walker Peter Baker

Current Mantid Usage at ISIS

Science Groups	Inspection	Live Data	Calibration	Correction	Reduction	Fitting	Modelling	Log Book	Publication
Reflectometry									
SANS									
SX Diffraction									
SX Spectroscopy									
Powder and DM Spectroscopy									
Disordered Mat. Diffraction									
QENS, DINS and Mol Spec									
Powder Diffraction									
Engineering and Imaging									
Muon Spectroscopy									
Training		n/a	n/a						n/a

Frequent Usage (> 50%)	
Occasional usage	
No usage	

Training

A common theme arising is that continuous training in Mantid at many levels is both highly appreciated when it occurs, and in further demand. This includes basic training for students and instrument scientists in addition to more in-depth training involving python scripting.

Both the ISIS Muon Training Course (bi-annual) and the ISIS Neutron Training Course (annual) use Mantid as standard - though other standard software used at ISIS is also included in these courses. Two important suggested improvements in training provision are:

1) The publication of an ISIS training schedule, including basic and specialist training activities would be appreciated.

2) The incorporation of e-learning problems and activities into the Mantid training activities may well significantly enhance basic Mantid training for the PhD intake, and across European institutions.

Individual Science Group Reports

Reflectometry

Instruments:
SURF, CRISP, POLREF, INTER, OFFSPEC

Main Contacts:
Tim Charlton and Owen Arnold. Some contact with reflectometry group at SNS, ISIS and SNS have different requirements - data analysis methodologies.

Other Software in use:
OpenGenie, python and Visual Basic scripts used for data reduction. Experimental setup and visualisation in EPICS.

Harmonisation:
User experience is identical on all instruments other than OffSpec - where science use cases are sometimes very different. Work now ongoing to bring OffSpec into closer harmony.

User Model:
Users generally leave with XYE files of reduced data. Physics users (magnetism) tend to install Mantid. Would prefer model where all users leave with Mantid installed, with hard links to external modelling software. Soft Matter users may need extra training.

Comparison of Mantid to Alternative Software:
Advantages:
- Cross-platform - suits users from different communities
- Instrument Definition Files - now well adapted to reflectometry

Disadvantages:
- Problems with loading times - esp. of nexus files.
- Graphics quality is less than state-of-the-art
- Screen clutter is a problem

Mantid Requirements List:
Short-term:
- fix needed for event mode filtering
- table based GUI for data reduction
- Harmonisation of IDFs and reduction procedures across instruments (i.e. OffSpec)
- Assessment of SNS GUI interface for use at ISIS

Mid-term:
- Reduction of off-specular data
- Combination of QxQz maps (VATES?)
- Compatibility with EPICS for IDFs
- Linkage with control software is important (Mantid on NDX machines)
- Statistical analysis of running datasets
- Seamless iterative scanning.

Long-term:
- Seamless integration of modelling packages - which would sit outside Mantid

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Small-Angle Neutron Scattering

Instruments:
LOQ, SANS2d, LARMOR, ZOOM

Main Contacts:
Steve King, Anders Markvardsen and Peter Parker. Sit down meeting between SANS group and Mantid developers each 2-3 months. Good interaction with SNS as well as ILL and NIST over several areas.

Other Software in use:
SASVIEW for fitting. Python-based (C++) built on all OS and supported by NIST. SNS/ISIS/ILL all helping with development. X-ray sources involved. Mantid team helps with the development of SASVIEW, but group could do with extra staffing effort for this.

Excel/SigmaPlot for publication quality graphs

Harmonisation:
User experience is identical on all instruments.

User Model:
Normally users leave with reduced data. Many take away raw data - unknown how many use Mantid at home.

Comparison of Mantid to Alternative Software:
Advantages:
- Can support event mode experiments which is not possible with other software

Disadvantages:
- Data reduction is slower now
- Capability of Mantid is now only “as good as Collette”
- Slow in event mode.
- Massive ticket list (109 items)

Mantid Requirements List:
Short-term:
- improved event file loading (and especially adding) speed
- enhanced graphical visualisation including Azimuthal averaging in SliceViewer
- “MultiPlot” visualisation of raw data
- Some data appears with zero error and non-zero intensity. This is incompatible with SASView, and incorrect. Major bug.
- More batch reduction capability

Mid-term:
- Treatment of GISANS data - strong overlap between this and off-specular reflection
- (Deadtime corrections) - unknown level of problem
- inclusion of “dark counts” - Cd runs
- Stitching of data sets at different instrumental configurations

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Single Crystal Diffraction

Instruments:
SXD, WISH, ALF

Main Contacts:
Pascal Manuel, Owen Arnold and Martyn Gigg. VATES acceleration meetings. Perceived lack of communication of changes causes problems. No regular meetings.

Other Software in use:
C++ / python script for Monte Carlo diffuse scattering calculations, plot-able in Mantid. Fullprof and GSAS supported. JANA supported. SHELLX supported

SXD2001 used exclusively on SXD. ALFnew used almost exclusively on ALF.

Harmonisation:
User experience is completely different on each instrument.

User Model:
Very different on each instrument. Users often leave with HKL list - but not in the case of diffuse scattering where analysis is user led. ALF data generally not used. No user demand for Mantid on SXD. ALF generally run by ISIS scientists - move to Mantid is desired.

Comparison of Mantid to Alternative Software:
Advantages:
- Mantid is de-facto sole option on WISH. But other than this less capability than SXD2001

Disadvantages:
- Remote access model is not fit for purpose - graphics support
- Development of multi-dimensional data set visualisation is very slow
- Poor Linux support

- Poor usability of visualisation interfaces
- Slow progress - hence need for acceleration project.

Mantid Requirements List:
Short-term:
- improved data visualisation and reduction via multi-dimensional data interface
- Instrumental calibration would be within Mantid (WISH)
- New peak integration options needed - shoe-box, line, etc.
- Avoid conversion to **Q** before integrating
- Comparison of Mantid and SXD2001 performance as benchmarking exercise
- Translation of ALFnew interface into Mantid

Mid-term:
- polyhedral shape dependent absorption corrections. (something which SXD2001 has now).
- Extinction corrections
- least squares fitting for profile matching purposes

Single Crystal Spectroscopy

Instruments:
MERLIN, MAPS, LET

Main Contacts:
Alex Buts embedded in excitations group. VATES acceleration meetings on regular basis. Alex collects requirements directly at group meetings. SNS - interactions are improving. (re. VATES meeting)

Other Software in use:
Horace (Matlab) - single crystal 4D data analysis. Mslice (Matlab) on LET, Merlin and sometimes MAPS - 3D single crystal analysis. TobyFit on MAPS fitting of spin-wave models with instrumental resolution convolution — slight take-up. “No” fitting provided on MERLIN/LET.

Harmonisation:
User experience is quite different on each instrument. Alex Buts now working on single user reduction script for all direct geometry spectrometers.

User Model:
Users log in to do remote data analysis and reduction on linux machines “Rutherford” and “Chadwick”. Very occasionally users take data away (normally in reduced .sqw format) and work on local machines provided enough computing power is available. “ease” of access to linux resources for users is a major sticking point.

Comparison of Mantid to Alternative Software:
Advantages:
- Mantid is able to correctly handle non-orthogonal axes which is a functionality missing from Horace.
Disadvantages:
- Mantid is somewhat slower than LibISIS predecessor, though event mode only possible in Mantid
- Usability problem with (unfinished) software
- Paraview graphics are not as good as Matlab
- Extremely slow on windows platforms
- Less group interaction and control than with Horace

Mantid Requirements List:
Short-term:
- Stop using Mslice - one less program to support. i.e. bring Mantid usability up to MSlice level
- MAPS to go over to Mantid calibration
- Rob (and Helen) to translate LET and MERLIN calibration routines to Mantid.
- Harmonisation of “iliad” script and auto-reduction

Mid-term:
- Move from Horace to VATES - seamless transition required (i.e. same user interaction)
Long term:
- Harmonisation with SNS is important long term aim.
- Tobyfit reproduction in VATES is needed for integration of fitting. Big hurdle to climb. Essential for long term use.
- Connection to modelling software (e.g. McPhase, CASTEP)

Powder and Disordered Materials Spectroscopy

Instruments:
MARI, MERLIN, MAPS

Main Contacts:
Alex Buts embedded in excitations group. Martyn Gigg for SliceViewer interface and legacy scripts written by Jon Taylor

Other Software in use:
Dave - NIST developed MSlice clone (IDL). MSlice (Matlab)

Harmonisation:
User experience is quite different on each instrument. Mantid used almost exclusively on MARI and in conjunction with MSlice on MERLIN / MAPS.

User Model:
Users generally leave with reduced ".spe" files (in nexus format). Mantid often installed on user laptops for MARI users, where size of the data-files is tractable.

Comparison of Mantid to Alternative Software:
Advantages:
- Mantid is able to correctly rebin the data (MSlice has incorrect algorithm to do this)
- Single platform for both data correction and reduction avoiding switch between Mantid and Matlab
- Scriptable interface which MSlice doesn't support
- availability of (in principle) absorption corrections

Disadvantages:
- Qti graphics are not as good as Matlab
- MSlice is more intuitive to use for non-experts
- DM spectroscopy needs multiple scattering corrections, and sophisticated absorption corrections

Mantid Requirements List:
Short-term:
- Stop using Mslice - one less program to support. i.e. bring Mantid usability up to MSlice level
- Harmonisation of "iliad" script and auto-reduction

Long term:
- Harmonisation with SNS is important long term aim.
- Connection to modelling software (e.g. CASTEP, polyCINS code)

Disordered Materials Diffraction

Instruments:
GEM, SANDALS, NIMROD

Main Contacts:
Nick Draper is main contact. (Anders initially developed IDF files for both NIMROD and SANDALS)

Other Software in use:
"JournalViewer" for log inspection. Java calibration routine written by Alan Soper, Gudrun performs data correction and reduction - this via a new Java interface. Code sustainability assured through 3 group members. Gudrun used widely in the DM community (including ILL and future use at SNS likely). EPSR (Soper) is used for data modelling. Mantid used extremely rarely (only for Neutron Training Course)

Harmonisation:
User experience is identical across instruments.

User Model:
Users generally leave with reduce XYE data. Gudrun is well trusted in the community - as a sophisticated “black box” solution. Only demand for Mantid comes within the neutron training course.

Comparison of Mantid to Alternative Software:
Advantages:
- None
Disadvantages:
- Current code is quick to run easy to use and trusted. Mantid lacks these features.
- Mantid does not include tried and tested multiple-scattering and Placzek (inelasticity) correction capability. DM needs high level of data correction.
- Large effort (from DM group) would be needed to bring Mantid to same level as Gudrun / EPSR.
- No motivation for/from users to switch away from Gudrun
- Unwillingness to lose control over software provision within the group.

Mantid Requirements List:
none

QENS, Deep-Inelastic Scattering and Molecular Spectroscopy

Instruments:
IRIS, OSIRIS, LET, TOSCA, MAPS, VESUVIO

Main Contacts:
Sanghamitra Mukhopadhyay looks after the coordination of requirements for the Molecular Spectroscopy Group. Group has benefited from the involvement of various Industrial Placement students. Martyn Gigg is main Mantid Group contact. Spencer Howells looks after QENS analysis software in Mantid. Weekly meetings held with Mantid Group. Strong contact with SNS (Basis).

Other Software in use:
Dave (NIST) sometimes used for QENS analysis. Old legacy code on VESUVIO currently used, but to be replaced imminently. MSlice and Dave commonly used on OSIRIS for magnetism experiments.

Harmonisation:
User experience is identical across each experiment class - i.e. QENS, Mol Spec. For VESUVIO, process of “Mantidisation” from legacy code continues. Strong harmonisation also with SNS.

User Model:
User meetings used to gather requirements. GUI's on TOSCA IRIS and OSIRIS, scripts on VESUVIO. Ascii files taken away. Mantid commonly installed on users laptops. (ascii not

used on VESUVIO). Group proactive in supporting users (e.g Luis Carlos Pardo - Bayesian analysis) usage of Mantid. Extensive Mantid user manuals written by the group aiding use of Mantid across group instruments.

Comparison of Mantid to Alternative Software:
Advantages:
- Mantid is single user correction, reduction and fitting user program.
- In standard use at ISIS and SNS
- Much better than other codes for infrequent users
- Python much more current than Fortran
- Harmonisation across instruments

Disadvantages:
- Documentation is not updated regularly enough. Particularly with the fitting functions.
- Often there are problems with stability of Mantid (some releases are buggy). Timing of releases could be better to check for bugs.
- need reasonable Multiple scattering and absorption corrections to be incorporated. (these are under-developed)
- Graphics ok - but not publication quality. "Cheap version of origin"
- Drive to expand seems to take precedence over stability.

Mantid Requirements List:
Short term:
- Prioritise VESUVIO - convert existing data reduction routines (and instrumental calibration routines) to Mantid format.
- Interface with CASTEP.
- Inclusion of multiple scattering.
- Improve plotting and GUI quality and integration of 3rd party software for QENS.
- Enhance Bayesian analysis routines

Mid-term:
- Robust and standard multiple scattering frameworks and sample self-attenuation corrections.
- Better and publication quality figures
- Better and wider use of 3rd party routines with seamless integration.

Powder Diffraction

Instruments:
POLARIS, HRPD, GEM, WISH, PEARL, INES

Main Contacts:
Martyn Gigg is main contact for Mantid locally. Strong contacts with the SNS via Pete Peterson. Powder routines written originally by Aziz Douad-Aladine. But some time ago.

Other Software in use:
Gudrun (Soper) and RMCProfile (Tucker) are used for total scattering experiments. Mantid not usable here for same reasons as given in the Disordered Materials section. Some total scattering software from Diamond. GSAS and Fullprof used for data modelling.

Harmonisation:
User experience is similar on most instruments (using Aziz's script based routines) but not WISH or PEARL which use their own script based routines. Total scattering experiments (mostly GEM and POLARIS) look very different. No current plans to further harmonise. POWGEN and SNAP use Mantid in similar way at SNS.

User Model:
Users generally leave with GSAS / Fullprof input files, or dye files for total scattering experiments. Mantid interface is all script based - demand to move to more GUI based interaction model. Plan in place to move to GUI interface to Gudrun (reading and plotting Gudrun files

Comparison of Mantid to Alternative Software:
Advantages:
- Mantid is well supported and maintained.
- Old software as fallen out of use and no longer works
- Sequential processing works well
- Mantid is cleverer and extendable (IDF files)

Disadvantages:
- Poor fitting interface in Qti
- Communication and training needs to be improved
- Poor stability - problems appearing between releases. Lack of science case testing.
- Slow loading of .nxs files - something to do with "history"
- Shifting priority lists are communicated badly - need oversight into what is being worked on and what is being dropped

Mantid Requirements List:
Short-term:
- improved stability and backwards compatibility
- "generic sample shape" absorption and multiple scattering corrections - **this is essential for absolute normalisation (total scattering) and vanadium corrections (powder diffraction).** Both these for divergent beams**.**
- Work needed to update Aziz's original scripts (all written in early days)
- Improve peak fitting interface and output in standard format
- Load files without "history" or "log" data
- Improve Mantid stability on PEARL (keeps crashing

Mid-term:
- Reference manual as single pdf file to aid script writing

- More Mantid training
- “stacked dataset” parametric multi-plotting as function of pressure/temperature, etc.

Engineering and Imaging

Instruments:
ENGIN-X, IMAT

Main Contacts:
Arturs Bekasovs was main contact. An (unknown) new person has been assigned. Patchy integration of the engineering requirements into Mantid, and patchy communications. (new student - Lottie). Federico working on imaging.

Other Software in use:
OpenGenie covers all current use cases on ENGIN-X - followed by data modelling generally in GSAS. Mantid occasionally used for “non-standard” operations.

In the future, IMAT will be the only instrument at ISIS doing imaging experiments. Mantid in combination with other software (ImageJ, AVIZO and others) will be used to analyse this.

Harmonisation:
Only one instrument in current use. Whatever is in use on ENGIN-X will move over to IMAT.

User Model:
Users are generally not crystallographers, and hence rely a lot on in-house instrument scientist support for data analysis. GUI interfaces preferred.

Comparison of Mantid to Alternative Software:
Comparison not straightforward as Mantid not used. “instrument view” occasionally proves useful (e.g. single crystal alignment). However, lack of support for OpenGenie and the possible of development of new algorithms in python/Mantid makes the move to Mantid highly desirable for the Engineering team. By the look of it, all of the ingredients required for data processing on ENGIN-X that currently exist in OpenGenie, also exist in Mantid.

Mantid Requirements List:
Short-term:
- Reproduce current OpenGenie reduction interface
- Remote data analysis (similar to excitations group)
- Instrumental calibration routines (which mirror current OpenGenie ones) to be incorporated
- GUI interface highly desirable
- Mantid interface to proprietary imaging software (in common usage at X-Ray sources)
- Large (> 100 Gb) data sets need to be supported (3d tomography)

Mid-term:
- Ability to deal with two crystallographic phases simultaneously
- Bragg-edge analysis (for imaging data)
- Pole figures for the analysis of surface texture (could be via hard link to proprietary codes)

Muon Spectroscopy

Instruments:
MuSR, EMU, HiFi, ARGUS, CHRONOS

Main Contacts:
Main interaction via Anders. Works well - Mantid team is responsive to requirements. Steve Cottrell is muon Mantid coordinator.

Other Software in use:
WiMDA (Francis Pratt) and OpenGenie. Origin or similar used for publication quality plots. Usage of WiMDA likely to continue due to popularity with a number of groups - and is a useful algorithm development platform in the group. Mantid is used > 50% of the time.

Harmonisation:
Each instrument uses same Mantid interface (as long as same version of Mantid is installed on each instrument).

User Model:
GUI interfaces are generally preferred by the users - Mantid used in both script and GUI formats. Users generally leave with raw data and either a copy of WiMDA or Mantid at their home institution / on laptop.

Comparison of Mantid to Alternative Software:
Advantages:
- Open-source and cross-platform
- Easy to include fitting functions - less of a black box solution than WiMDA
- Downloadable for all users and easy to install

Disadvantages:
- Graphics are rather low quality
- New Mantid versions and updates sometime result in non-functioning of muon interfaces and functionality
- Mantid projects don't save properly - exact state of Mantid is not saved.

Mantid Requirements List:
Short-term:
- Better integration/usability of MaxEnt Fourier analysis
- Multi-histogram fitting (this is being rolled out in version 3.3

- Tiled displays of data
- GUI for Fourier analysis (FFT and MaxEnt)
- “Avoided Level Crossing” analysis functionality to be added (automatic point addition)
- Dynamic Kubo-Toyabe is missing!

Mid-term:

- Interface to DFT code (Gaussian) for HF coupling calculations and muon sites
- Modelling of spectra via Monte-Carlo methods / equations of motion