Report on usage of Mantid at ISIS

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Remit

- To gather current Mantid take-up and usage information across ISIS science activities.
- To assess whether the short-term requirements set out in the previous usage report (Jan 2015) were addressed.
- 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

- The stability of Mantid has improved over the last 12 months. Similarly, many of the speed issues highlighted in Jan. 2015 have been addressed (though issues remain in the SANS and Powder Diffraction groups).
- Signs of much improvement in the area of neutron diffraction
  - In the “vates simple interface”
  - In the interaction with the engineering and imaging instrumentation group
  - initiation of the process of updating of the original powder diffraction routines

  However, replacement of the old powder diffraction scripts is taking far too long.
- SANS has benefited from some improvements in mantid usability this year
- Usage of Mantid has increased across ISIS - with the addition of the engineering and imaging group, and on VESUVIO
- No instrument group feels particularly under-supported (unlike 12 months ago) - reflecting a greater level of informed strategy. However, there is still a very varied interaction model between Mantid and each of the instrument groups. Some groups appear to engage very strongly while others appear more passive with sometimes poor levels of communication.
- Most instrument groups use Mantid in combination with 3rd party software - with the dividing line set subsequent to data reduction. Modelling and fitting activities are generally performed with proprietary software, or software developed in-house by instrument groups. Some instrument groups (notably excitations) have some difficultly in identifying where this line should be drawn.
- Some sticking points remain where Mantid development is slow - notably in Reflectometry, Muons and much of Spectroscopy there is slow progress in many of the requirements set out in Jan 2015. Some concentration on spectroscopy may now be required (or in the near future).
- The disordered materials group doesn’t use Mantid - and is increasingly convinced that it will never do so. Lack of implementation of basic neutron scattering corrections in Mantid is partly to

blame for this.

- Some instruments have multiple science use cases, and these require different Mantid approaches to harmonise across instrument groups. e.g. the QENS GUI interface in IRIS/ OSIRIS and LET should be identical. Similarly, the diffraction routines on OSIRIS should be the same as are used on POLARIS, GEM and PEARL.

- Potentially useful features of Mantid (such as auto-reduce, live data, alternative interfaces such as IP notebook) are perhaps under-utilised. This is at least in part due to under communication of these utilities.

- Response time to short-term requirements in Mantid is slow. Some improvements in some areas are mirrored by a lack of real progress in others.

- Common issues with Mantid:
  - **Lack of absorption and multiple scattering corrections**. This was highlighted last time, and little progress has been achieved.
  - **Waterfall/Stack plots.** Common requirement between diffraction and muon groups. Likely to be useful to other groups.
  - **Low quality graphics.** Again highlighted last time. This forces users to use proprietary software when it should not be strictly necessary (e.g. use of origin in the muon group)
  - **Lack of usability.** The two main issues here are; multi-dimensional visualisation (which is not widely used other than by WISH and MARI) and the instability of saving Mantid project files.

Mantid Team

Nick Draper (Tessella)	Karl Palmen (ISIS)
Martyn Gigg (Tessella)	{Alex Buts} (ISIS)
Owen Arnold (Tessella)	{Lottie Greenwood} (ISIS)
Roman Tolchenov (Tessella)	Lamor Moore (ISIS/ESS)
Anton Piccardo-Selg (Tessella)	Michael Hart (ISIS/ESS)
Matt Jones (Tessella)	Shahroz Ahmed (ISIS, Student)
Federico Montesino-Pouzols (ISIS)	Thomas Brooks (ISIS, Student)
Raquel Alvarez Baños (ISIS)	Elliot Oram (ISIS, Student)
Anders Markvardsen (ISIS)	Matt King (ISIS, Student)

Science Groups Survey

This survey is based on meetings held with representatives of each of the science group areas between the 4th Dec 2015 and 7th Jan 2016. These groups do not follow ISIS instrument groups in all cases

Each group was asked to give an appraisal of the use cases and frequency of use of Mantid on instruments in their science area. The groups were asked to give their view of interactions and communication with the Mantid team at ISIS, to assess improvements and ongoing issues, to assess how their requirements from 12 months ago have been addressed, and to update their requirements for the coming short- (~12 month) mid- (~2 year) and long-term (~5-year) requirements.

Science group	Participants
Powder Diffraction	Ron Smith Steve Hull
Single Crystal Diffraction	Pascal Manuel Matthias Gutmann Silvia Capelli Steve Hull
Engineering and Imaging	Winfried Kockelmann Shu Yan Zhang Joe Kelleher Saurabh Kabra
Total Scattering	Helen Playford
Disordered Materials Diffraction	Tristan Youngs Daniel Bowron
Small-angle Neutron Scattering	Steve King Richard Heenan John Webster
Reflectometry	Max Skoda John Webster
Powder and Disordered Materials Spectroscopy	Tatiana Guidi Duc Le
Single Crystal Spectroscopy	Helen Walker Devashi Adroja Russell Ewings
Quasi-elastic scattering, Deep Inelastic Scattering and Molecular Spectroscopy	Sanghamitra Mukhophadyay Matthew Krztiniak Felix Fernandez Alonso Giovanni Romanelli
Muon Spectroscopy	Steve Cottrell Adrian Hillier

Current Mantid Usage at ISIS

Science Groups	Inspection	Live Data	Scripting	Calibration	Correction	Reduction	Fitting	Modelling	IP Notebook	Publication	Auto-reduce
Powder Diffraction											
SX Diffraction											
Engineering and Imaging											
Total Scattering											
Disordered Mat. Diffraction											
SANS											
Reflectometry											
Powder / DM Spectroscopy											
SX Spectroscopy											
QENS, DINS and Mol Spec											
Muon Spectroscopy											

Frequent Usage (> 50%)	
Occasional usage	
No usage	

Key:

Inspection	Use of instrument view, single spectra, etc.
Live data	Use of live data interface in Mantidplot
Scripting	Use of mantid to write user-scripts, and “on-the-fly” analysis routines
Calibration	Use off mantid in instrument calibration (e.g. PSD detectors, vanadium measurements)
Correction	Use of mantid in data correction (background subtraction, normalisation, masking, etc.)
Reduction	Use of mantid in “reduction” of data (change of units, focussing, rebinning, etc.)
Fitting	Use of Mantidplot fitting interface (or other) for analytical fits
Modelling	Use of mantid for numerical modelling, or as interface to 3rd party software
IP-Notebook	Use of the Python notebook interface
Publication	Use of mantid for production of publication ready graphics
Auto-reduce	Use of the auto-reduce interface based on a mantid script

Powder Diffraction

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

Main Contacts
Martyn Gigg is working on multiple scattering and absorption corrections. Federico is working on Aziz's old routines in an attempt to understand them and convert them to the new api. Since Aziz and Matt Tucker have both left ISIS, Ron Smith is now the contact for powder diffraction, with Helen Playford looking after the PDF analysis side.

Other software in use
OpenGenie is still used for quick inspection of data (live-data is not used). Data modelling is done with standard Rietveld refinement software (GSAS, Fullprof, Topas) and Mantid interfaces adequately with these. PDF analysis done with Gudrun and RMCProfile.

Harmonisation
GEM, POLARIS and HRPD share common Mantid routines (written in the early days of Mantid by Aziz Daoud Aladine). PEARL and WISH use their own Mantid scripts (developed by Bill Marshall and Matt Tucker for PEARL and Pascal Manuel and Laurent Chapon for WISH). Total scattering experiments on GEM and POLARIS look very different and hardly use Mantid. Group plans to further harmonise reduction scripts across the suite. No contact or harmonisation with the SNS planned or desired.

OSIRIS uses different routines and different methodology to the other powder diffraction instruments. Harmonisation of this is desirable.

User Model
This is unchanged from last time. Users ask for GSAS/Fullprof/XYE files which they then analyse on their own machines, using their preferred software package. Data modelling not provided or necessary from Mantid. Current script based interaction with Mantid seems to be accepted as the normal mode of operation. Not much push for GUI interfaces.

Comparison of Mantid to Alternative Software
No alternative to mantid for data focussing. Old OpenGenie and Ariel routines no longer in use. Stability of Mantid is seen to have improved over the past 12 months.
Ongoing problems:

- Lack of absorption and multiple scattering corrections which used to exist in older reduction platforms (mentioned above)
- Lack of "stack plots" - these were available and good in GENIE II
- Stability issues still exist when reading .nxs files.

Mantid Requirements List

Delivered since Jan 2015

- Improve Mantid stability on PEARL, and elsewhere
- Load files without history or log data

Short term

- "generic sample shape" absorption and MS corrections - essential for absolute normalisation of total scattering and standard vanadium corrections - **ongoing, good progress made**
- Replacement of Aziz's scripts for GEM, POLARIS and HRPD - **ongoing. Perhaps best solution is to base new scripts on current PEARL scripts.**
- add "stack plot" capability to Mantid - **ongoing and now short term**

Single Crystal Diffraction

Instruments
SXD, WISH, ALF
(SXD does not use Mantid at all)

Contacts
Owen Arnold still main point of contact in Mantid team. Pascal Manuel lead scientist, and Silvia Capelli tasked with testing capabilities of Mantid on SXD in the future. Pascal sometimes attends the VATES acceleration meetings.

Other Software in use
(WISH) C++/Python scriptable “DiffMag” program for analysis of diffuse scattering on WISH - integrated with Mantid. Fullprof and GSAS commonly used for refinement.
(SXD) SXD2001 IDL code run on SXD, Mantid not used. Jana and ShelX used for modelling of data. Matthias supports own suite of diffuse scattering analysis programs. “Diffuse” code sometimes used.
(ALF) “ALFnew” in almost exclusive use. Mantid used very occasionally

Harmonisation
The user experience is completely different on all 3 instruments

User Model
Users leave with corrected HKL intensity lists, or more collaborative analysis model in the case of diffuse scattering. Mantid used for fitting when Rietveld analysis not possible (e.g. thin film analysis)
(WISH) Analysis takes place on local machine (normally) - isiscompute used occasionally by users from their home institutions.
(SXD) Still no user demand for Mantid on SXD.
(ALF) Move to Mantid desirable, but ALFnew familiar to part time users, and sophisticated enough to deal with most use cases.

Comparison of Mantid to Alternative Software
Direct comparison of SXD2001 to Mantid has been desired for a long time, but has not taken place as yet. This is partly due to the fact that Mantid operates in Q-space exclusively for single crystal analysis while SXD2001 operates in detector space. A detector space option is required in Mantid before any meaningful comparison can take place.
Ongoing problems:
- SXD instrument team unaware of Mantid capabilities
- User model problematic on WISH (updated of local linux machines - FIT issue)
- Dealing with multiple crystallites
- Lack of ability to analyse data in detector space

Mantid Requirements List

Delivered since Jan 2015
- Improved data visualisation (VSI improvements)
- Better data loading times
- Instrumental calibration now fully integrated in Mantid
- New peak integration options installed (shoe-box, line, etc)

Short term
- **Avoid conversion to Q before integration (work in detector space) - ongoing and crucial for comparison with SXD2001. Likely to be crucial for MaNDi at the SNS.**
  (NB - these routines apparently exist at the ILL and may naturally be added to Mantid if/when the ILL joins the project)
- Comparison of SXD2001 and Mantid - **not started**

- Polyhedral shape model absorption corrections (currently existing in SXD2001) - **ongoing. Nick Draper has looked at this with a project student. ILL have scripts to do this in Mantid. Relevant SXD2001 code given to the Mantid team to translate**

Mid Term

- Wavelength dependent extinction corrections - **ongoing. This exists as a kind of fudge in Mantid now. Needs further discussion and improvement**

Engineering and Imaging

Instruments:
ENGIN-X, IMAT

Main Contacts:
Federico Pouzols is contact for both imaging and engineering applications. Much better contact with Mantid now - Saurabh Kabra and Federico meet on a (nominal) bi-weekly basis. The Engineering and Imaging scientists are happy with the current Mantid interaction, and "don't want to change" the current contact.

Current Usage of Mantid
Mantid used for occasional "instrument view" applications. New GUI has been developed by Federico for reduction of ENGIN-X data. This could be adapted to cover other powder diffraction use-cases, and will include interface to new GSAS2 software, and event mode filtering. (currently 3 use-cases for powder diffraction analysis; ENGIN-X, HRPD/POLARIS/GEM, WISH). Federico also developing IMAT interface which will find and correct image data and send to 3rd party applications for display and manipulation. Some script development work using python is undertaken using Mantid.

Other software in use
This is unchanged in the last 12 months. OpenGenie still in use on ENGIN-X, followed by data modelling in GSAS (version1). Using Image-J, AVIZO and Octopus for imaging applications (IMAT).

Harmonisation
Only one instrument currently in use. ENGIX-X and IMAT will be fully compatible. (for strain-imaging)

User Model
As before, users are generally not crystallographers. Therefore, simple software interfaces are required, and generally a high degree of local contact support during data analysis and reduction.

Comparison to alternative software
The new GUI will provide identical functionality to the current OpenGenie interface - but with the prospect of much more (including improved and more sophisticated data correction, event mode filtering, etc). Scripting in python now superseding OpenGenie.
Much current discussion of the lines of demarkation between Mantid and proprietary imaging software. But team happy with current direction of the imaging project in Mantid.
GUI interfaces possible in Mantid - not with OpenGenie.

Mantid Requirements List
Delivered since Jan 2015:

- Reproduce current OpenGenie reduction

Short-Term:

- Implement ENGIN-X GUI (first users Dec 2015) - **ongoing**
- Implement IMAT GUI - interface to 3rd party software and data handling - **ongoing**

- Improved peak fitting **- new**
  - New profile shapes (Bragg-edge fitting) **- moved from mid-term requirement**
  - Improvements desired in stability
  - Improvements desired in usability of the fitting interface
- Interface to GSAS2 **- new**

Mid-Term:

- Pole figure diagram production (for analysis of surface texture in materials) - **ongoing**
- Implementation of Mayers-like multiple scattering corrections in vanadium calibration - **new**

Total Scattering (polycrystalline)

Instruments
GEM, POLARIS

Main Contacts
Helen Playford is coordinating this within the crystallography group - working closely with Matt Tucker who recently moved from ISIS to the SNS. Martyn Gigg is main contact within the Mantid team.

Current Usage of Mantid
Mantid used for focusing data (Aziz Douad-Aladine routines - same as used for powder diffraction). This is appropriate for GSAS file output (Bragg peak analysis). Occasionally Mantid is used for taking quick FFT transforms to create PDF (pair distribution function) datasets. Some calibration constants retained by Gudrun are lost in the GSAS files created by ADAs reduction scripts.

Other Software in Use
Gudrun used for focussing, corrections and background subtraction - appropriate for analysis of peak + diffuse scattering. STOG used to produce PDF output. RMCProfile used for fitting of both the GSAS and the Gudrun output files. This is complicated by the fact that the calibration constants are lost in the GSAS output file.

Harmonisation
The user interaction is identical on both GEM and POLARIS. Likely future strong harmonisation with the total scattering science activities at SNS.

User Model
Users reduce data on-site with Gudrun - which can be slow, but not prohibitively so. RMCProfile is commonly run on local university clusters, or remotely using the SCARF cluster. Some users are largely autonomous, but given eh more complex reduction and analysis workflow involved in total scatter, some extensive student training is required to get to this stage.

Comparison to Alternative Software
Gudrun provides stable interface to background, attenuation, multiple scattering and inelastic corrections that are so far unavailable in Mantid. Mantid provides a level of adaptability (on-the-fly analysis) that is not possible with Gudrun. Both analysis packages provide a reasonable user experience but harmonisation required to ensure a better fit between them.

Mantid Requirements List
Short term

- Wrapper interface to Gudrun within the current Mantidplot interface. Should be a joint ISIS/ SNS effort.
- Calibration content of Gudrun and Mantid output files should be identical
- Replacement of legacy ADA routines with more transparent and up-to-date scripts. Ideally following the PEARL/WISH methodology.

Long term
- Move fully to Mantid - removing dependency on Gudrun for more sophisticated data correction

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Disordered Materials Diffraction

Instruments
GEM, SANDALS, NIMROD

Main Contacts
No contact between DM group and Mantid team. Alan Soper used to go to the Scientific Steering Committees but doesn't intend to interact further, and will not go to the next meeting.

Other software in use
Most use cases on DM instruments are looked after by Gudrun, via Java interface (open source-Alan Soper). Code sustainability is assured in-group. Gudrun used widely in the DM community (including the ILL and future use at SNS likely). OpenGenie used occasionally in group. EPSR (Alan Soper) most often used for data modelling. Usage of Mantid is restricted to instrument view 1 day a year (during ISIS neutron training course).

Harmonisation
User experience is identical across all instruments.

User Model
Most users use Gudrun / EPSR. None use Mantid.

Comparison of Mantid to alternative software
Mantid currently does not offer a viable alternative to Gudrun, which is quick, easy and trusted. Ongoing problems are:
- No tried and tested multiple scattering corrections, crucial in DM diffraction
- No Placzek (inelasticity) corrections
- Extremely large effort (and mostly from the DM group) would be needed to bring mantid to level of Gudrun / EPSR

The disordered materials group has no Mantid requirements

Small-Angle Neutron Scattering

Instruments
SANS2d, LOQ, LARMOR, ZOOM

Contacts
Anton Piccardo-Selg in now main Mantid contact having taken over from Peter Parker and then Anders Markvardsen. (apparently 6 Mantid contacts in as many years). Steve King and Richard Heenan are LSS group contacts, though with the retirement of Richard due in February 2016, more group effort in Mantid is acknowledged to be necessary.

Other Software in use
SASview (international collaborative software project administered by NIST and with partners from ILL, ESS, ISIS). SASview is python based open source and cross-platform.
FISH software still being used for modelling. Proprietary software for pub quality graphics.

Harmonisation
User experience is identical on all SANS instruments

User Model
Users normally leave with fully reduced data (ascii files which are compatible with SASview). Many take home raw data and have Mantid installed on their machines. Some difficulties arise when dealing with large data sets from SANS2d.

Comparison of Mantid to Alternative software
No alternative to Mantid on SANS instruments (event mode)
Ongoing problems:
- Slow performance appears still to be an issue on windows computers.
- mantid workflow in scripts is slower than it should ideally be
- Ongoing and massive list of tickets - focus is on firefighting rather than important strategic thinking in future directions.

Mantid Requirements List

Delivered since Jan 2015
- Improved event file loading (and adding) speed
- Zero-error and non-zero intensity incompatibility with SASVIEW
- More batch reduction capability

Short term
- enhanced graphical visualisation including azimuthal averaging in SliceViewer - **ongoing, no progress**
- “MultiPlot” view of different runs in instrument view / SliceViewer / Colour Fill Plot. - **ongoing, no progress**
- Improvement of usability of SliceViewer - **new**
- Re-write of old SANS scripts (under the GUI) is desirable - **new**
- Need continuity of support from lead Mantid developer (currently Anton) - **new**
- Fully scriptable batch reduction capability (moving forward from that already achieved) - **new**
- Possibility of inclusion of batch reduction table interface used for reflectometry - **new**
- propagation of x-errors through Mantid routines is required - **new**

Mid term
- Treatment of GISANS data - ongoing usability problems with SliceViewer - **ongoing**
- Stitching together different runs (with detectors at different positions) - **ongoing**
- Dead time corrections (unknown how to proceed with this) - **ongoing**
- Multiple scattering and absorption corrections should be implemented - **ongoing**
- Scanning interface for looking at event mode data in order to quickly identify relevant parts of the dataset - **new**
- Improved publication quality graphics in Mantid (e.g. control of line thickness, fixed aspect ratio and size of plot, proper histogram plots).- **new**

Reflectometry

Instruments
SURF, CRISP, INTER, OFFSPEC, POLREF

Main contacts:

Don't know who Mantid contact is. Currently change in personnel in the reflectometry team with Tim Charlton (who was the main Mantid user in the team) leaving. Max Skoda will probably adopt the role of Tim in the future.

Other software in use:
Software other than Mantid is used for modelling and 2d (off-specular) manipulation. These programs are either user-provided fitting / modelling programs, or Matlab based fitting program in the case of off-specular. (off-specular reflectometry is around 10% of the user programme on INTER and POLREF). Rascal modelling software (with MD compatible output) is often used. OpenGenie is used for instrumental scanning data.

Harmonisation:
User experience is identical on SURF and INTER. POLREF also uses same or similar routines, but largely using the python notebook interface. OFFSPEC uses different routines customised for that instrument. The reflectometry group is desirous of achieving greater harmonisation between their instruments, and recognises that this will take some internal discussion to sort out. The "table entry" routines developed in the last year are in use across INTER, SURF and CRISP - not POLREF or OFFSPEC. This should be adapted to suit all reflectometers in the near future.

User Model:
Users leave with XYE files of corrected/reduced data. The reflectometry group are interested in pursuing a user model similar to that of the excitations group - that is to use a web interface to local (ISIS) reduction computers. This would aid version and platform control for Mantid and stability. High performance computing is not an initial concern.

Comparison of Mantid to Alternative Software:
No alternative to Mantid now up to fitting level for specular reflectometry.
Ongoing issues:

- Residual problems with fundamental incompatibilities between multi-period data and .nxs files.
  - Live-data is sluggish (and can lead to Mantid crashing)
  - Outputted .nxs files are x100 the size of the input data
- No solution for 2d (off-specular) visualisation - sliceviewer not user friendly. Matlab preferred.
- Stability and uniformity of Mantid between platforms and versions is an issue (lower than desired level of scientific unit testing)
- Save mantid projects is unreliable. Graphs are not re-created properly
- Cannot save graph templates

Mantid Requirements List:

Delivered since Jan 2015

- table based GUI for data reduction
- usage in tandem with control software (labview / EPICS)

Short term

- Fix needed for event mode filtering and multi-period loading - **ongoing**
- Harmonisation across instruments (IDFs , routines and user interface) - **ongoing**
- New features needed for GUI interface (Multidetector processing (2d), live data, polarization analysis) - **new**
- Inclusion of event workspace reduction in table interface - **new**
- Assessment of SNS GUI interface for use at ISIS - **ongoing and extremely slow**
- Reduction of 2d and off-specular data - **ongoing - no progress**
- Scripts needed for inspection of scan data - **new**

Mid term

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- Combination of 2d Qx-Qz maps - **ongoing - no progress**
- Improvements required to slice-viewer if it is to be made usable for reflectometry applications (scaling issues, buggy usage, non-editable preview plot) - **new**

Long term
- Integration of modelling packages (such as Rascal) - **ongoing**

Powder and Disordered Materials Coherent Spectroscopy

Instruments
MARI, MERLIN, LET, MAPS, IRIS, OSIRIS

Contacts
Alex Buts is main point of contact for the group (embedded). Duc Le and Tatiana Guidi are group contacts.

Other Software in use
MSlice (Matlab), and DAVE (developed at NIST - IDL)

Harmonisation
User experience is similar on each direct geometry instrument (LET, MERLIN, MAPS and MARI) - same script developed by Alex Buts is used on each, though sometimes with a wrapper developed by Russell Ewings is used (MARI and MAPS). On IRIS and OSIRIS a GUI based initial reduction is used.

User Model
As is the case for single crystal spectroscopy, users analyse data (on instrument and from home institution) on isiscompute. Older users still have issues with account creation on this system, but other than the that system is working well. Instrument scientists actively encourage users on MARI (where the bulk of the powder spectroscopy is done) to use Mantid for data reduction - rather than MSlice, however this approach has mixed success with the powder spectroscopy user community

Comparison of Mantid with alternative software
There is now no alternative to initial data correction and conversion than Mantid. Mantid competes with MSlice (DAVE) for data visualisation and reduction.
Ongoing problems:
- SliceViewer is at a significantly lower usability level than MSlice
  - Overplotting is difficult and time consuming
  - Graphical dragging of cuts is very rarely used
  - slower to use than Mslice
- Lack of absorption and multiple phonon corrections for time-of-flight data (something which used to be available)
- Problems with slow divergence of scripts unless controlled (i.e. harmonised user experience diverging slowly over time)
- Continued buggy usage of auto-reduce web interface

Mantid Requirements List

Delivered since Jan 2015
- Harmonisation of “iliad” script and auto-reduction (though auto-reduction not used yet. Period of test usage of auto-reduction will commence soon hopefully)

Short term
- Need to stop supporting and using MSlice. **This requires MSlice emulator to be written for Mantid platform. Same requirement as for SX spectroscopy**
- Better harmonisation now required between direct geometry and indirect geometry instruments (same script interface) - **new**

Mid-term
- Full absorption and multiple scattering corrections required (for generic geometries) - **new**

Long-term
- Connection to modelling software (e.g. CASTEP, SpinW) - **ongoing**

Single Crystal Spectroscopy

Instruments
MERLIN, MAPS, LET, OSIRIS

Main Contacts
Alex Buts embedded in the excitations group. VATES acceleration meeting held on regular basis (ISIS/SNS).

Other software in use
Horace (Matlab) - 4D data analysis, visualisation and fitting. MSlice commonly used for 3D visualisation (2 Q directions - static crystal). TobyFit on MAPS - fitting of spin-wave models with instrumental resolution. Modelling using SpinW and McPhase undertaken on piecemeal basis by users. Some support of phonon modelling using CASTEP.

Harmonisation
User experience is now fully harmonised on MERLIN, LET and MAPS (same mantid scripts and reduction software, developed by Alex Buts). OSIRIS users also use Mslice, and use a GUI based interface for initial data correction and unit conversion.

User Model
This has undergone a significant process of change this year. Users now use the isiscompute cluster for Mantid, Mslice and Horace operation - both on the instruments and from their home institutions using the “NoMachine” web interface. Users reduced data is kept in “RB folders” associated with their experiments, and all users on the experiment have access to these folders. After initial teething problems this system is now working well.

Comparison of Mantid to Alternative software
No alternative to mantid for initial data inspection and correction since LibISIS deprecated. Mantid speed issues with respect to older software have been addressed with some success. Horace though has caught up with Mantid in terms of analysis of non-orthogonal axes.
Ongoing problems:
- Usability - this is why users and instrument scientists continue to prefer Horace
- Graphics - these are generally acknowledged to be better in Matlab, and not at all good in QT or Paraview
- Though still slow on windows machines, there are no longer used in the group.
- Still less group interaction with Mantid than with Horace (not surprising given that Horace is developed by the group)
- Slow development of Horace script emulator despite much increased group engagement. Unless accelerated this could lead group to abandon Mantid as a platform for analysis and visualisation.

Mantid Requirements List

Delivered since Jan 2015
- Harmonisation of “iliad” script and auto-reduction - **both delivered though auto-reduce not used**

Short-term

- Must stop using Mslice - this may require building MSlice emulator within Mantid framework - **ongoing**
- Move from Horace to VATES - seamless transition required (i.e. same user interaction) - **ongoing**
- Tobyfit reproduction in VATES is needed for integration of fitting - **ongoing**
- Mantid calibration to be used on all instruments (requires translation of exiting matlab routines into Mantid) - **ongoing - no progress**

Mid-term

- Connection to modelling software (e.g. McPhase, CASTEP, SpinW)

QENS. DINS and Molecular Spectroscopy

Instruments
IRIS, OSIRIS, LET, TOSCA, MAPS, MARI, MERLIN, VESUVIO

Main contacts
Sanghamitra Mukhopadhyay coordinates the Mantid effort in the Mol Spec group, and Elliot Oram is dedicated to (and embedded in) this group. Martyn Gigg is the lead Mantid contact.

Other software in use
The group uses Mantid for much of its computing - up to and including data modelling and fitting, beyond the level of other groups at ISIS. However DAVE (NIST) is also sometimes used for fitting and visualisation. Development of DAVE is, however, slow and Mantid shows more scope for future development. DFT and Molecular Dynamics codes are commonly used (by users) and Mantid can read and use output from these codes (e.g. CASTAP and nMolDyn)

Harmonisation
Three distinct experiment classes are taken care of within the group. For QENS the user sees identical GUI interfaces on the indirect spectrometers, but not on LET, where the data reduction is script based. Similarly; a “push button” GUI is available on TOSCA for Molecular spectroscopy but not on the direct spectrometers where - again - scripts are used. Further harmonisation here is strongly desirable. VESUVIO uses script based reduction, and has no immediate requirement to move over to a GUI.

Diffraction data taken on OSIRIS is analysed in a different way to that on all other powder diffraction instruments (see powder diffraction).

User Model
“Push button” GUI interface essential for Mol Spec and QENS users - and should be extended to direct geometry instruments.

Users tend to install Mantid on laptops and home institute computers. Since Mantid is used for reduction, fitting and modelling (commonly), data is taken away in Mantid Project form. Sometimes ascii (or .spe, .gss) output used for import into fitting software (such as DAVE, GSAS). MD data visualisation tends not to take place in Mantid. For TOSCA, users take away xye files for use with proprietary software..

Absorption corrections using old QENS fitting code (from Spencer Howells) can only take place on Windows OS computers.

Comparison of Mantid to alternative software
No alternative to mantid for initial data inspection and correction. Fitting and visualisation capability is on a par with DAVE, which is preferred by some users. Last year a perception of a

lack of current documentation was flagged by the group, and large improvements have taken place in this area.
Ongoing problems:

- Still problems with stability and bugs. Scientific unit tests not compatible with GUI interfaces.
- Still lacking absorption and multiple scattering corrections (except for VESUVIO)
- Memory problems occur with VESUVIO data (proliferation of workspaces)
- Quality of the graphical output is still too poor to publish.

Mantid Requirements List

Delivered since Jan 2015

- Analysis of liquids/powder on VESUVIO is now done in Mantid (including resolution)
- Interface to CASTEP for density-of-states data.
- Implantation of Bayesian Analysis (FABADA) - publications produced.

Short-term

- Inclusion of absorption and multiple scattering corrections - **ongoing**
- Continued development of Bayesian analysis and CASTEP interface for S(Q,ω) (as opposed to DOS) - **ongoing**
- Harmonisation of OSIRIS powder diffraction routines - **new**
- Backwards compatible data analysis (for TFXA and old TOSCA) - **new**
- Q-dependent model interface to CASTEP is next stage - **new**
- Data masking capability for removal of spurions (user interactive) - **new**
- Continued transfer of VESUVIO routines (for single crystal, Y-space, calibration, etc) - **new**

Mid-term

- GUI streamlining to improve stability and transparency, and to render compatible with script operation - **new**
- Publication quality graphics (and movies) - **ongoing**
- Resolution deconvolution routines for TOSCA - **new**

Long-term

- Full implementation of resolution deconvolution across instrument suite. **- new**
- Full implementation of multiple scattering corrections **-new**

Muon Spectroscopy

Instruments
MuSR, EMU, HiFi, ARGUS, CHRONUS

Main Contacts
Raquel Alvarez Baños is now main contact in Mantid team taking over from Anders. Steve Cottrell looking after Mantid from the muon group. Frequency of meetings too low at the moment.

Other software in use
WiMDA (Francis Pratt) is used around 50% of the time for muon data analysis and reduction. OpenGenie is now used very little. Origin is used extensively for production of publication quality graphs, saving of data (in Origin project files), producing “squashograms”. Origin is popular among many muon user groups, and is acknowledged to be more user friendly and intuitive than Mantid. Some MonteCarlo modelling performed using Quantum (James Lord) which is now included in the Mantid script repository.

Harmonisation
Each of the EU side instruments (EMU, MuSR and HiFI) uses the same user interface and GUI. Some residual problems with version control of Mantid between instruments. RIKEN side

instruments (ARGUS and CHRONUS) use almost exclusively WiMDA. This situation is likely to continue.

User Model

Users see GUI interfaces mainly, and not much demand is perceived for scripting interfaces. Users generally leave with .nxs files, together with local installed copies of Mantid or WiMDA. Many users take away save Origin project files (seemingly, many users have licensed copies of Origin). Perceived difficulty in saving ascii files from Mantid (as not included in GUI).

Comparison of Mantid to alternative software

Mantid and WiMDA are currently used about equally for muon data correction and reduction. Origin is used for fitting and graph production (and project saving)

Mantid vs. WiMDA;

- Mantid is unable to analyse transverse field muon spectroscopy measurements. (in the frequency domain). WiMDA therefore is used in these situations.

Mantid vs. Origin

- Origin can reliably save project files - this is very unreliable in Mantid at the moment (plot windows not appearing
- Mantid's user interface is less intuitive
- Mantid lacks publication quality graph templates

Mantid Requirements List

Delivered since Jan 2015

- Multi-histogram global fitting
- Tiled displays of data
- Inclusion of the Dynamic Kubo-Toyabe function in the fitting interface
- Avoided level crossing analysis
- Modelling of spectra via Monte-Carlo methods / equations of motion(Quantum)

Short term

- Better integration of MaxEnt / Fourier (frequency domain) analysis - **ongoing**
- GUI required for multi-histogram fitting - **new**
- GUI required for frequency domain analysis - **ongoing - no progress**
- Smooth transition required from Mantid to Origin (send data) - **new**
- Need for Mantid to save projects reliably and 100% reproducibly **- new**
- Automatic point addition required for avoided level crossing data (auto-reduce) - **new**

Mid-term

- interface to "Gaussian" DFT modelling software - **ongoing**
- Inclusion of dipolar field calculations for determination of muon stopping sites - **new**
- WaterFall plots for multi-histogram plotting (similar to those required for powder diffraction) **- new**