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SSI/Mantid - Collaboration Review

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Contents

Executive Summary

The Mantid project[1], a large international collaboration between the Science and Technology Facilities Council (STFC) and the US Department of Energy (DoE), provides a framework for the analysis of neutron scattering and Muon spectroscopy data. It represents a collaboration between 4 of the major international neutron centres and the Tessella commercial company. At the time of writing, the project has been running for 9 years, and a review of the collaboration, use and development around the software was requested from the Software Sustainability Institute to feed into a general review of the project's strategic science objectives, governance and software quality.

This report provides an analysis of results from a questionnaire sent to scientists and users of Mantid, which was open from the end of September to early November, and received a total of 78 responses. The greatest proportion self-identified as senior instrument scientists, with the most popular instrument on which responses were based was WISH. The means by which respondents use Mantid is almost equally divided between computers at the facility, logging into a facility remotely, and installed on computers outside of the facility, with only a very small proportion using autoreduction on its own. Nearly half of users[2] access Mantid on both Windows and Linux machines, and only a quarter of all users make use of Mantid on Mac OS X.

In general, the Mantid project appears to be doing very well in servicing the needs of its end-users, particularly given the scale of the collaboration and the diversity of science being conducted and analysed using the software. The effort and skill required to organise such a large-scale project should not be underestimated, and tts processes and practices, and the project itself, have evolved over time to be generally very effective in servicing those needs.

The general findings from analysing the responses, noting areas for improvement, were as follows:

- ***For general data reduction, respondents are generally satisfied with data reduction timeliness and quality***, although there is some improvement to be made regarding the ease of plotting data. There is also a strong call for improved data processing and data access speed, despite the general satisfaction with timeliness.
- ***A clear majority of respondents are satisfied with how Mantid integrates with their scientific workflow***, although a substantial majority need to perform at least some pre-processing and/or post-processing on their data, which is perhaps to be expected. The biggest barriers are the general stability issues with Mantid, learning to perform data plotting and visualisation, and lack of documentation for basic tasks and conducting technique-specific tasks.
- ***In terms of the software itself, the most popularly used and most important features of Mantid are MantidPlot and using Mantid within Python.*** In general, respondents report high ratings for usability, functionality and particular scripting support, although, again, there is clear room for improvement in terms of reliability and visualisation, as well as

[1] http://www.mantidproject.org
[2] Note: users could select multiple OSs.

a need for improved ease of use in terms of a cleaner GUI for specific scientific applications and a simpler command set.

- ***A significant proportion agree that Mantid's documentation is useful, with many reporting it's also comprehensive and contains the right amount of technical information.*** A significant proportion are able to find the documentation they are looking for, although nearly as many have encountered some of greater difficulty. There is a strong request for more worked examples that are applicable to user scenarios, and improved user documentation for routine uses of the software and the expected behaviour of algorithms, with an ability to more easily search algorithms by their purpose.
- ***The biggest barriers to learning how to use Mantid is the need for better tutorials and more worked examples***, already noted in terms of documentation, and are represented in a comparatively large number of comments.
- ***In terms of maintenance and technical support, by far the greatest proportion of users only encounter occasional problems when using Mantid, and only occasionally need help to resolve them***, although a notable proportion encounter problems most of the time, and a similar proportion need help most of the time to resolve issues. This is unsurprising given the necessary breadth of functionality and complexity of Mantid. Nearly half of respondents indicated the information available to solve issues themselves was sufficient, and nearly a third indicated they found the process of registering requests for support generally easy. Half indicated the timeliness for incorporating technical fixes into releases was either good or excellent, whilst the majority rated the timeliness for incorporating new features was generally good or fair. The quality of fixing technical issues was also rated very highly, and the quality of new feature development is generally fine. There are also a notable number of requests of delivery of technique-specific support, which is also noted previously as a barrier to learning to use Mantid.
- ***For project communication, direct email and face-to-face meetings are by far rated the most highly, and most popular, methods of communication with the Mantid team***. In general, most respondents agree that they are sufficiently informed about the project's activities, and there is strong agreement that the Mantid project has a recognisable and distinctive identity within its own user community.
- ***Nearly half of respondents have attended a training event, and the majority indicate intermediate-level skills training is the most important***. The organisation and information provided for training events was highly rated, as well as being useful in attendee's future work. There is some indication that there are not enough training events, although the is very strong agreement that there is adequate expertise available at respondent's sites. Holding science technique-specific training courses is suggested.
- ***In terms of project governance, nearly a quarter have attended a Scientific Steering Committee meeting, and there is very strong agreement that the project's activities are well aligned with its scientific objectives, and that the project is generally able to make effective decisions.*** However, a substantial proportion are not familiar with how the project is governed and a notable proportion indicate they are unaware of how features requests are generated and put into the development programme. The most common request is for greater communication between the Scientific Steering Committee and stakeholders.

There are also a number of common themes that emerged strongly from comments *across* the categories (in order of overall frequency):

- ***Better documentation and support,*** particularly for new users, including technique-specific courses and support, documenting the expected behaviour of algorithms and allowing for better algorithm discovery (mentioned in general general data reduction, integration with scientific processes, concerning the software itself, documentation, barriers to use, maintenance and support, and training). An aspect that is very strongly noted is that there should be more worked Mantid examples and tutorials that can be readily applied to scientific activities (mentioned in regards to documentation, barriers to use, and training).
- ***Improved resilience against crashes*** (mentioned in general data reduction, integration with scientific processes, and concerning the software itself).
- ***Faster data processing and data access speed*** (mentioned in general data reduction, integration with scientific processes, and concerning the software itself).
- ***Improved data plotting*** (mentioned in general data reduction, integration with scientific processes, and concerning the software itself).

It should be noted that the issues related to documentation of algorithm discoverability and description, task-oriented documentation and tutorials, were also highlighted in the Institute's Development Review report, a technical assessment which was conducted independently of this review. An aspect raised in that report that is directly related to these issues is the website, which whilst comprehensive and of high quality, requires reorganisation of its material which is often difficult to find. The Mantid tutorials are also very useful and well constructed, but need to go further, needing to provide basic instructions for many use cases - and worked examples - which is strongly echoed in this assessment. This could leverage Sphinx for documentation and code examples, which is currently used by the project to automatically test code fragments and help reduce maintenance overhead of the material.

Generally, there is a common high-level request for greater cohesion between the Mantid team and its users which is achievable in a number of ways, which should be investigated.

Firstly, greater communication between the Scientific Steering Committee (SSC) and users is seen as potentially beneficial. Greater transparency through dissemination of request and decision-making procedures and meeting minutes should be considered, as well as involving greater input from front-line instrument scientists and users in decisions, working towards a publicised roadmap for future releases. This would, however, incur additional effort in the area of governance which is already seen as an expensive process. Making use of efficient survey mechanisms to provide feedback on SSC plans may ameliorate this additional burden. This was also echoed, at a lower level, in the *Development Review*, where development practices and processes, whilst well defined, are not always documented.

At a wider scale, and echoed in the comments, it may make sense to consider a general annual user meeting across the facilities to discuss development progress, promote networking and a sense of shared community, and collect and discuss requirements for roadmapping at a wider

scale. A single yearly PMB meeting that is open to a greater number of representatives could also be considered, perhaps coupling it with, or holding it prior to, the annual user event.

The project's arrangement to have 1-2 developers aligned with each scientific group/technique area is commendable, reducing the risk of 'over the wall' development solutions that are inappropriate to end-user requirements. Additionally, taking into account a few key comments (one notes that the quality of support seems dependent on the instrument scientist), it may be beneficial to take this a step further and embed Mantid developers on experiments in-situ for a period of time. This would help them increase their understanding and appreciation for the underlying barriers faced by beamline scientists, and to provide in-situ training on using Mantid for their experiments to supplement existing training Mantid courses. If this were done for each experiment, this would have the added benefit of developing an even better foundation of scientific operational understanding across the Mantid developer team to inform design and other development decisions, and potentially allow instrument-specific support liaisons between the Mantid team and the scientists.

A notable observation regarding the balance between fixing issues and developing new features, is that fixing technical issues, whilst considered a more rapid and quality process, would seem to require comparatively greater attention and prioritisation compared to development of new features. This is a common problem with large-scale, multi-partner, long running scientific projects. As highlighted in discussions with Mantid developers, a great number of long-standing issues exist and are increasing, which was also observed in the *Development Review*, again highlighting the need for additional effort for issue management and resolution. Instituting issue re-prioritisation meetings between each scientific group and assigned Mantid developer(s) could potentially clear much older issues that are no longer relevant whilst highlighting those that are still important.

The project faces the obvious and common problem of limited effort, and prioritisation of that effort, to accomplish a wide range of tasks on a large-scale project. An option to consider to alleviate this situation is instituting official user or scientific champions across the wider collaboration, for specific techniques, algorithms or documentation, for example. Acting as a partially 'devolved' spokesperson and coordinator for their local group, they collate, channel, and regularly reprioritise requests and issues at a technical level. The benefits to Mantid are the offloading of some level of responsibility and effort - which in terms of issue management is a known problem - and for the champion, official acknowledgement of the role and possibly greater input into the development cycle. Added advantages are that it raises the level of requirements discussion, potentially reducing 'noise', and as more facilities join in the future, becomes a more scalable way of dealing with requirements.

1 Introduction

1.1 Overview

This report provides an analysis of results from the Collaborative Questionnaire[3] sent to scientists and users of Mantid, which was open from 29 September to 4 November, and received 78 responses. The questionnaire was structured around the 10 areas: general data reduction, integration with scientific working processes, the software itself, documentation, software learnability and barriers for new users, maintenance and technical support, project communication, training events, project governance and general comments. For each area, a number of quantitative questions to solicit opinions in that area were provided, as well as the opportunity to supply general comments for improvement.

1.2 The Mantid Project

The Mantid project[4], a large international collaboration between the Science and Technology Facilities Council (STFC) and the US Department of Energy (DoE), provides a framework for the analysis of neutron and Muon data. It represents a collaboration between 4 of the major international neutron centres:

- Rutherford Appleton Laboratories (RAL) in the UK,
- Oak Ridge National Laboratory (ORNL) in the US,
- Institut Laue-Langevin (ILL) in France,
- European Spallation Source (ESS) in Sweden / Denmark,

A company called Tessella[5] also forms part of this collaboration.

Mantid provides a framework to support high-performance computing and visualisation of materials data. Although it's been created to manipulate and analyse neutron scattering and muon spectroscopy data, it could be applied to many other types of data.

At the time of writing, the project has been running for the last 9 years and this year, they would like to review the project, both in respect of its strategic science objectives, governance and software quality. This assessment activity is intended to feed into that review process.

1.3 Structure of this Document

This document is structured around the structure of the questionnaire, addressing each of the areas introduced in section 1.1 generally in the order they were presented in the questionnaire. Each section provides a summary of the responses to the quantitative and qualitative questions.

[3] https://drive.google.com/open?id=0B5NCB6s6ow7kZ2hPdGNGMW9JQmM
[4] http://www.mantidproject.org
[5] https://tessella.com

The comments analysis collates the comments into common areas, listing key points brought up in specific comments. For a full record of comments for each area, see Appendix A.

2 Response Analysis

2.1 Questionnaire Response Summary

2.1.1 Responses by Primary Role

A total of 78 responses were received from the Collaborative Questionnaire. The breakdown of responses in terms of primary role is shown in Figure 1.

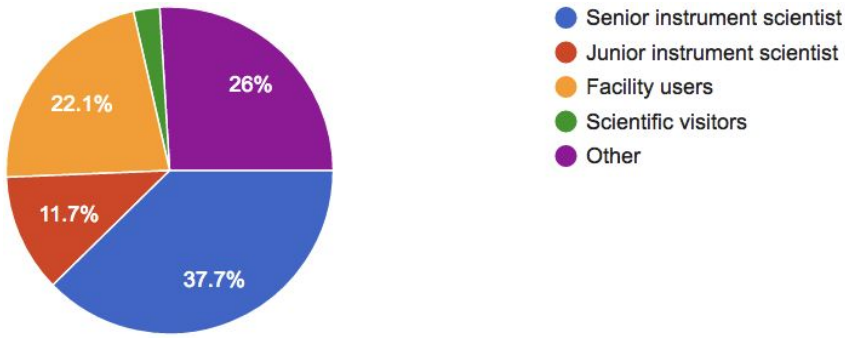

Figure 1. Breakdown of responses by primary role

In general, this would seem to indicate a reasonable collection of responses across those roles.

2.1.2 Responses by use of Mantid

Looking at how respondents use Mantid (see Figure 2), only a small proportion of users indicate they only use Mantid indirectly via autoreduction, whilst a significant proportion (25 respondents) indicate they use Mantid through 'Other', which represents a class of users who access and use Mantid via multiple methods.

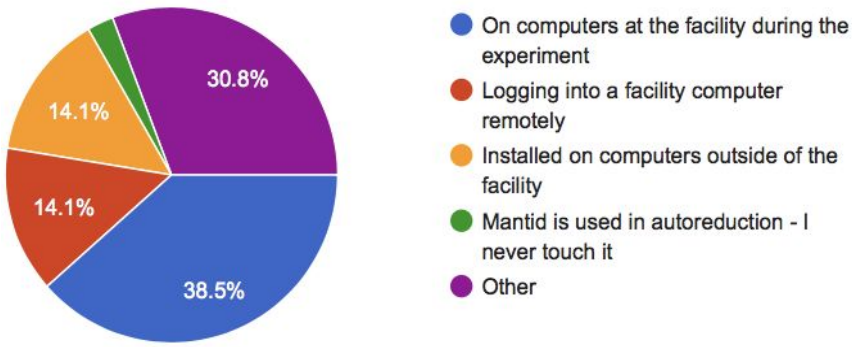

Figure 2. How do you use Mantid? (For those users providing a single method, or 'Other')

An aggregate view of how respondents use Mantid, also taking into account those respondents using multiple methods of accessing Mantid in the 'Other' category, is shown in Figure 3.

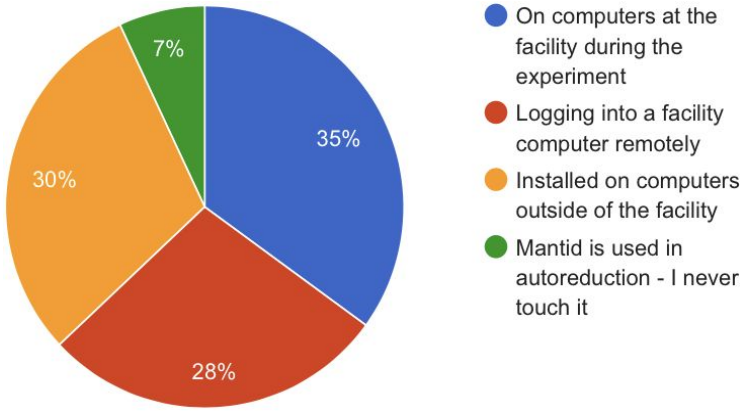

Figure 3. How do you use Mantid? (Taking into account respondents who use multiple methods to access and use Mantid)

Here we observe a far greater proportion of respondents using Mantid off-site, either remotely logging in, or having an installation elsewhere.

Figure 4 shows a breakdown of this 'multi-access' users group, and the combinations of access methods they employ.

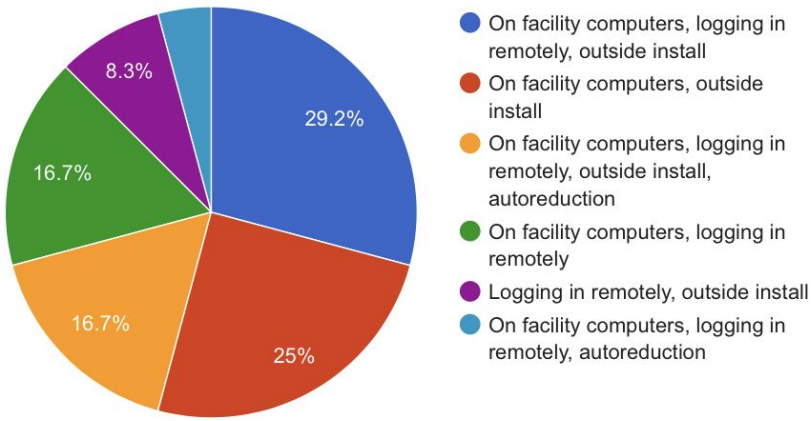

Figure 4. Breakdown of these 'multi-access' users, and the combinations of access methods they employ

The majority of multi-access users access facility computers together with an outside installation, perhaps logging in remotely.

In terms of the operating systems used by respondents (see Figure 5), the vast proportion of use is split evenly between Windows and Linux.

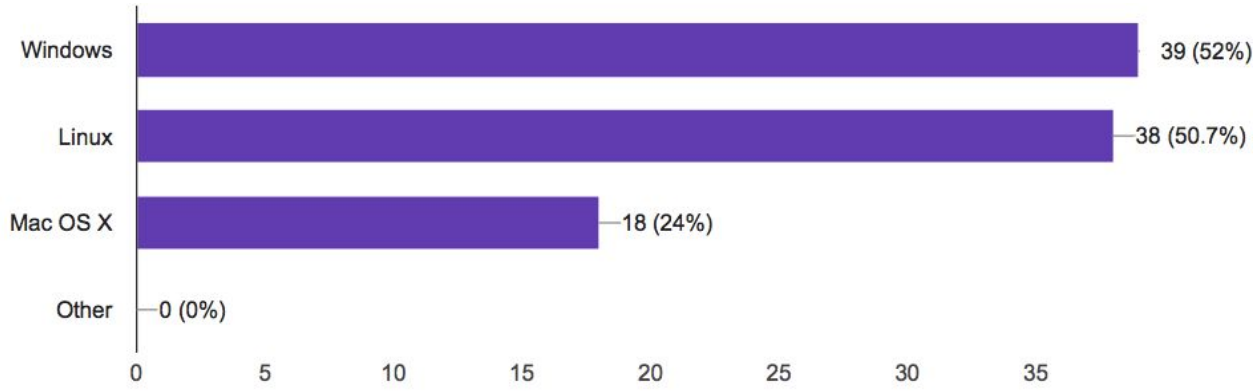

Figure 5. Operating systems used by respondents to run Mantid

2.1.3 Responses by Instrument

Figure 6 provides a breakdown of the instruments upon which they were basing their responses, with by far the greatest proportion completing the questionnaire for WISH.

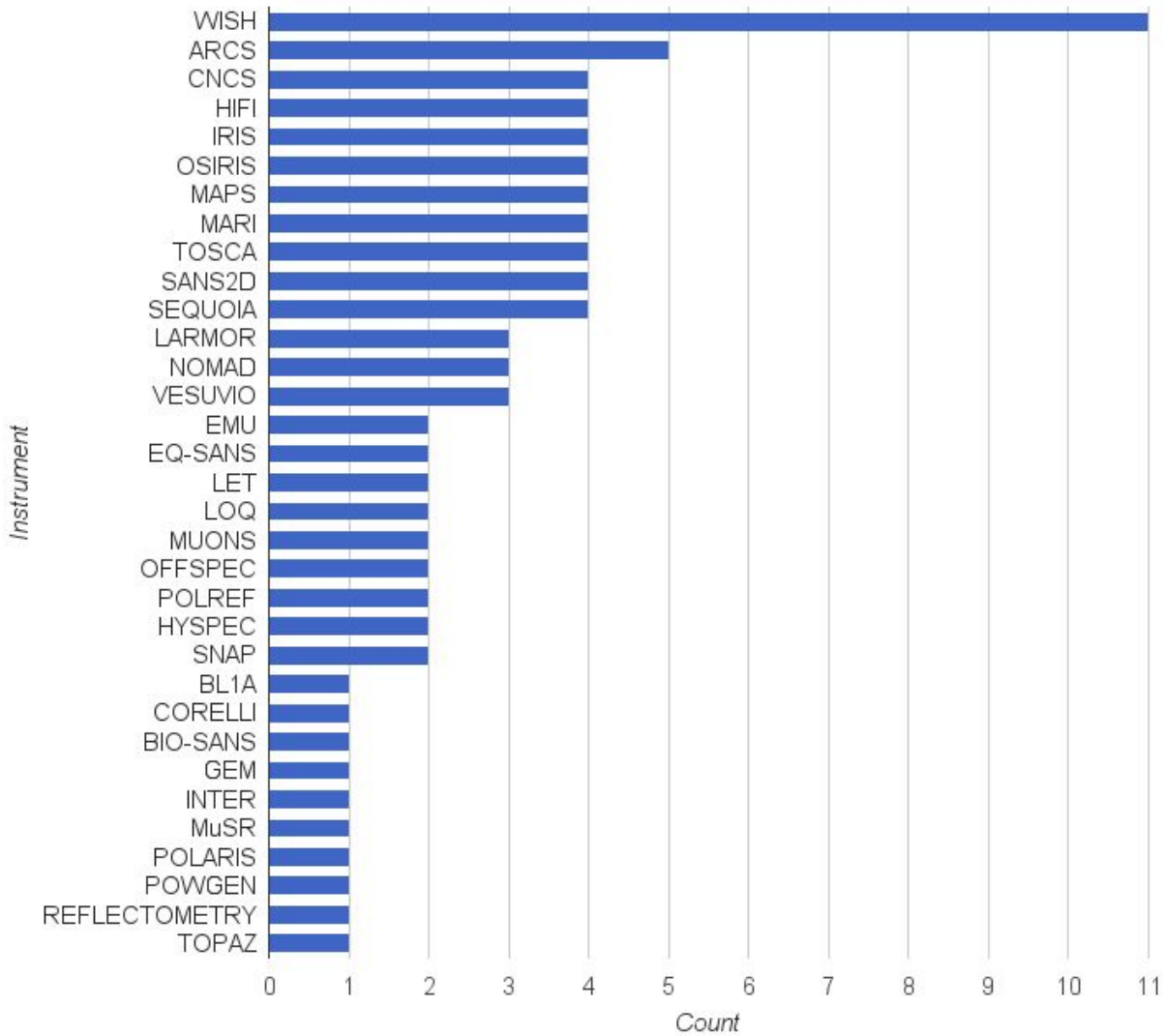

Figure 6. Breakdown of responses by instrument

2.2 General Data Reduction

Figure 7 shows the overall satisfaction with general reduction services, which indicates respondents are generally satisfied with data reduction timeliness and quality (although 5 indicate they are very unsatisfied with timeliness, which perhaps should be investigated). Comparatively, there are generally more respondents satisfied than unsatisfied regarding the ease of plotting data, although the level of dissatisfaction should be noted.

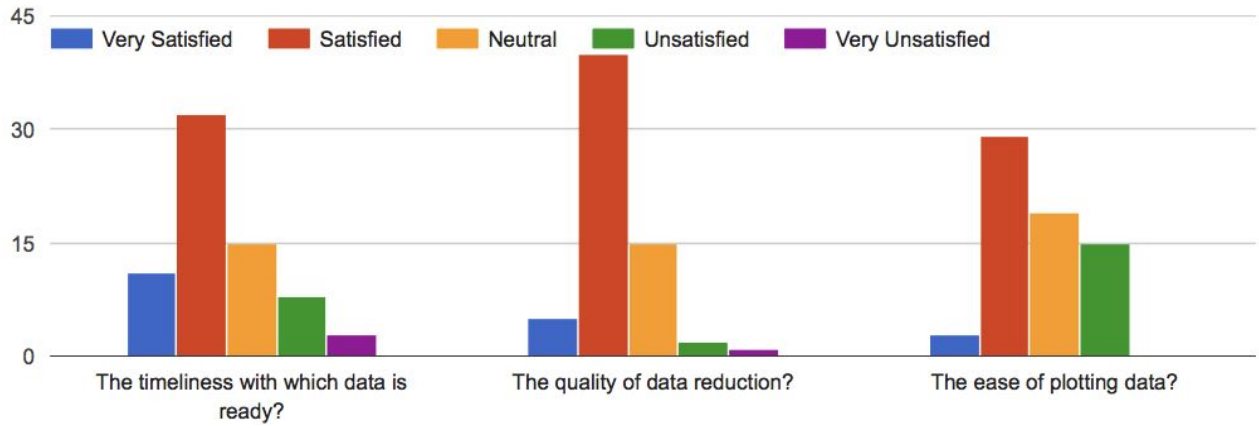

Figure 7. Satisfaction of respondents with timeliness, quality of data reduction and ease of plotting data

There were 53 additional comments on how data reduction could be improved; summarising the most common requests:

- **Data processing and data access speed needs to be improved, in some cases significantly** (including on-the-fly analysis, and for legacy instruments) [13 requests]
- **Better documentation and support for new users** (in particular, better documents on reduction options) [6 requests]
- **Improved resilience against crashes** [4 requests]
- **Improved user-friendly data plotting** (perhaps incorporating good default values and simples interfaces to change settings, and zooming and reading of datapoints should be simplified) [4 requests]
- **Improved corrections** (for multiple scattering and absorption) [3 requests]
- **A graphical user interface that works across all direct geometry instruments**, removing need for custom scripts for each instrument [3 requests]
- **Further automation for reduction** (for non-ISIS instruments, such as VESUVIO) [2 requests]

See Appendix A.1 for a full summary of comments.

2.3 Integration with Scientific Working Processes

Figure 8 indicates the respondent's' satisfaction regarding Mantid's integration with scientific working practices, with a clear majority either satisfied or very satisfied with this aspect.

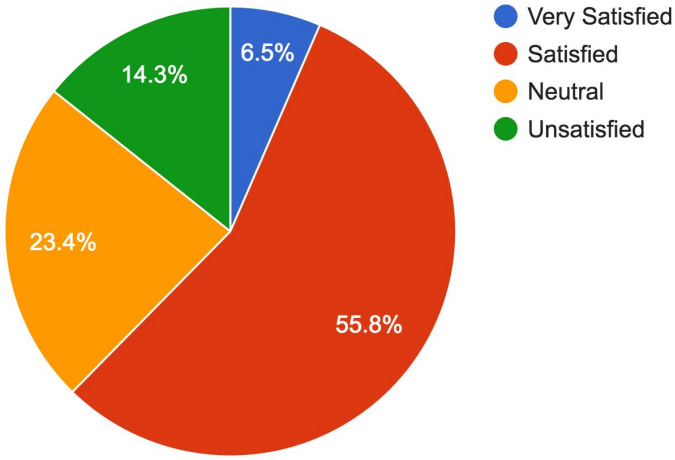

Figure 8. How satisfied are you with how Mantid integrates into your scientific working processes?

Figure 9 shows the extent to which respondents need to conduct additional pre- or post-processing on their data. A greater proportion need to perform post-processing, although perhaps that is to be expected, and is reflected in many comments received throughout the survey.

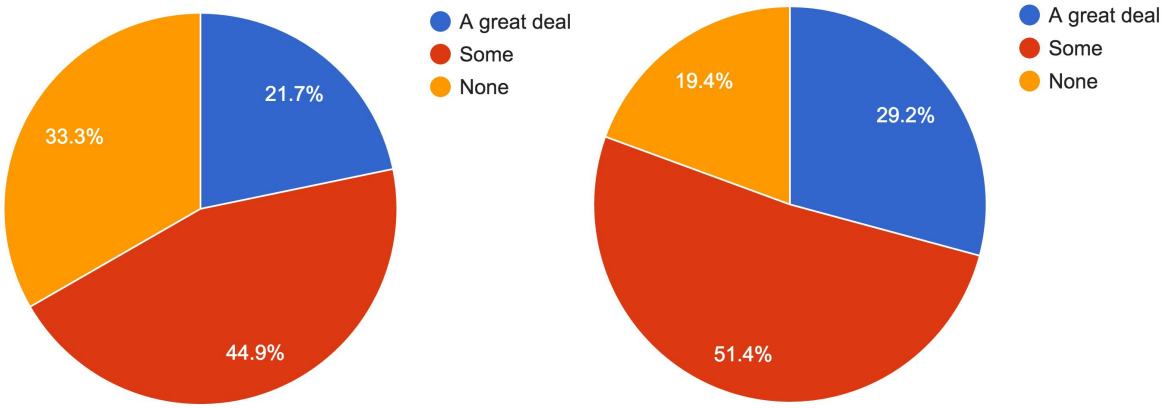

Figure 9. How much pre-processing (left) and post-processing (right) do you need to fit Mantid into your working processes?

There were 58 additional comments on barriers preventing better integration between Mantid and working processes; summarising the most common barriers:

- **General stability** (including when processing single crystal data, when using some of its algorithms in scripts to post process data) [9 responses]
- **Data plotting and visualisation within Mantid** (including plotting of direct geometry not being done within Mantid, difficult to learn, not able to produce Matplotlib figures within Mantid, often just do plotting in Python outside of Mantid) [7 responses]

- **Lack of user manuals** (including for basic tasks, plotting, inelastic neutron scattering with time-of-flight direct geometry instruments, lack of code examples) [6 responses]
- **Time taken to perform data reduction** (even for a single data set) [5 responses]
- **Algorithms changing from one version to another causing issues** (for example in reduction scripts arising from changed requirements for inputs to algorithms) [4 responses]
- **Need for more fundamental algorithms incorporated into Mantid** (including for adsorption and multiple scattering corrections, transformation to phonon density-of-states, better access to fitting algorithms with resolution effect incorporated) [3 responses]
- **Exporting data in a timely and helpful format** (including for use in Matlab, Fullprof (GEM and WISH), inability to output data in .nxs format directly from the workspace (WISH), use with simulation software) [3 responses]
- **The general complexity of Mantid** [2 responses]
- **How Mantid deals with displaying windows** (for example, it resets a lot of windows every time a data file is loaded, difficult to find certain windows) [2 responses]

See Appendix A.2 for a full summary of comments.

2.4 The Software Itself

In terms of how often respondents use each of the Mantid applications in their work (see Figure 10), we can see that virtually everyone uses both MantidPlot and Mantid within a Python script, although use of Mantid within an iPython/Jupyter notebook is low. Just over half of respondents use Mantid in autoreduction, albeit much less frequently than MantidPlot or Mantid scripting is used.

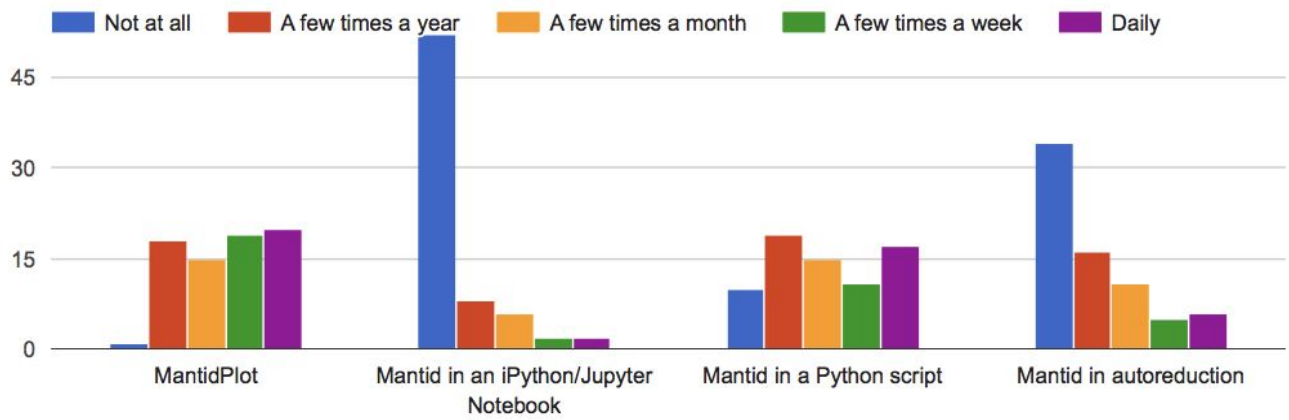

Figure 10. How often do you use the following applications?

Looking at the importance of these applications (see Figure 11), we see profiles of importance for MantidPlot and usage of Mantid within Python scripts which are broadly similar and indicate generally high importance regardless of frequency of use in both cases. For Mantid's autoreduction we also see relatively high importance despite lower frequency of use, whilst the importance of Mantid within iPython/Jupyter notebooks is generally consistent with its indicated frequency of use.

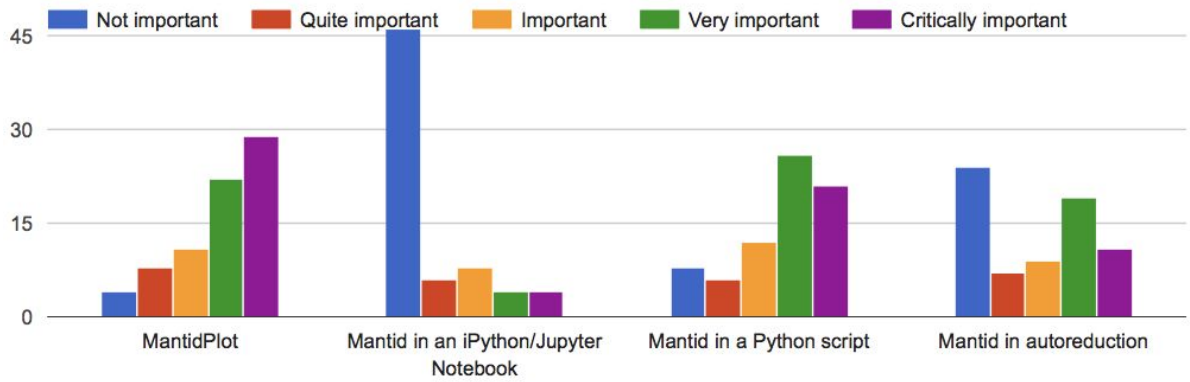

Figure 11. How important are the following applications in your work?

Looking at Figure 12, we see that the majority of respondents provided high ratings for usability, functionality, and particularly scripting support, and ease of installation is rated even more favourably. However, there is clear room for improvement in terms of reliability and visualisation capabilities, which is consistent with the analysis of comments shown in terms of barriers preventing better integration between Mantid and working processes (section 2.3), and how data reduction could be improved (section 2.2).

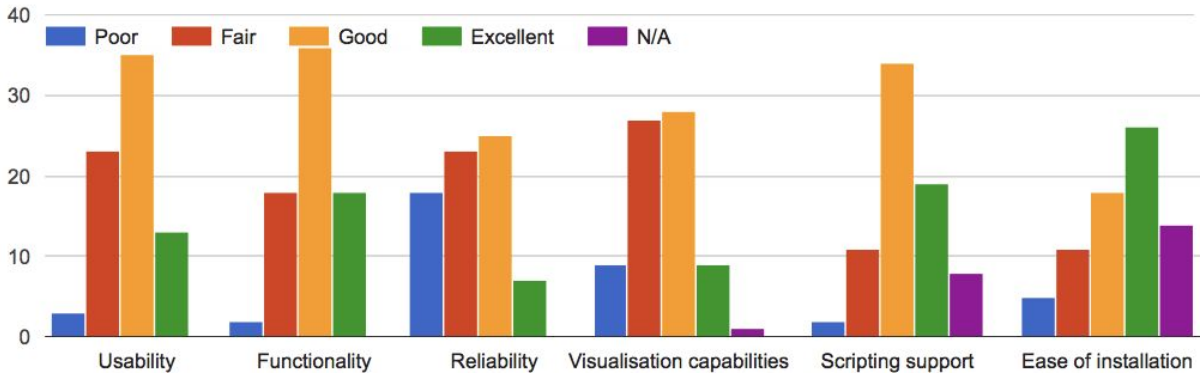

Figure 12. How would you rate the following aspects of Mantid for your purposes?

In terms of the frequency of software release (see Figure 13), the overwhelming majority either have 'No opinion' or consider the rate of releases 'Just right', with the remainder of results indicating a slight lean towards 'Too frequent'.

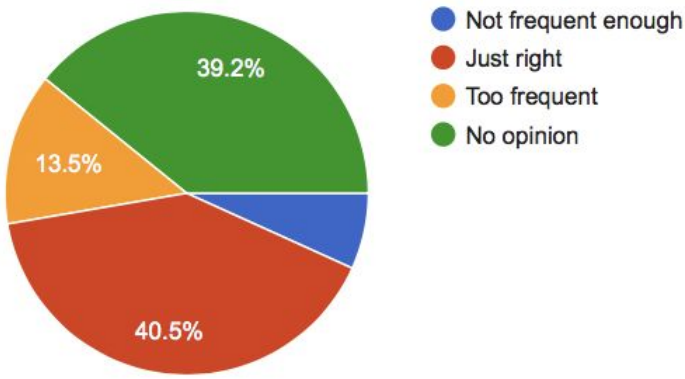

Figure 13. How would you rate the frequency of software releases?

There were 51 additional comments on requests for improvements to the software; summarising the most common:

- **Improved stability** (including improvement of system tests, reduction, MantidPlot, random crashes, better memory management for reliability, resolving bugs for table copy and paste, Mac stability) [18 requests]
- **Improved data plotting** (including simpler plotting, 3D plotting, easier integration of 2D/waterfall/3D plots, better quality figures for publication, line zooming is awkward, options of inspecting the plot need to be direct access of options for inspecting plots via shortcuts) [12 requests]
- **Improved ease of use** (including cleaner GUI interface for specific applications, a simpler command set, less reliance on GUI, universal GUI for direct geometry instruments, easier modifying of algorithms, easier visualisation of algorithm tree index) [7 requests]
- **Improved processing speed** (including SANS reduction, Catalog when selecting multiple files) [5 requests]
- **Improved fitting** (multi-peak, full pattern, pole figures, handling multiple datasets, background fitting) [4 requests]
- **Improved export capabilities** (for graphics, data, 2D maps from batch reduction (ISIS SANS), compatibility with fullprof) [3 requests]
- **Improved documentation** (including a user manual for scripting and built-in features, guide to setting up an instrument via instrument definition files, more contextual help) [3 requests]
- **Improved saving of projects** (including having previous settings and saved plots return when reloaded) [2 requests]
- **Improved integration with the iPython notebook** [2 requests]

See Appendix A.3 for a full summary of comments.

2.5 Documentation

A significant proportion of respondents agree or strongly agree that the documentation is useful (see Figure 14), with around a quarter agreeing or strongly agreeing that the documentation is comprehensive, and a just over a quarter agreeing that it contains the right amount of technical information to be useful.

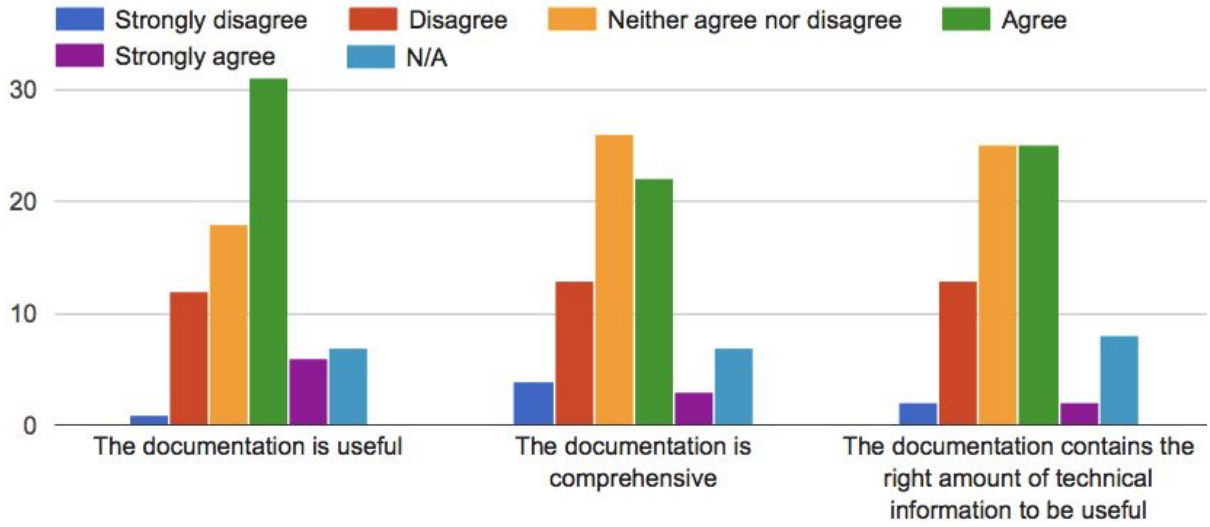

Figure 14. To what extent do you agree with the following statements concerning documentation (usefulness, comprehensiveness, technical information)?

Whilst a significant proportion of respondents are able to find the documentation they are looking for (see Figure 15), nearly as many respondents have encountered some or perhaps greater difficulty. Generally, the documentation is available in the right formats.

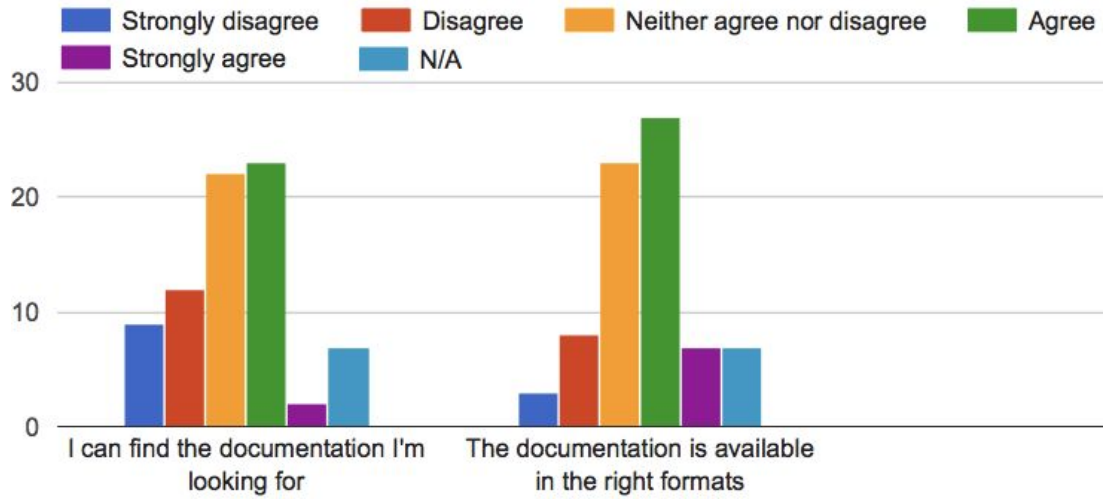

Figure 15. To what extent do you agree with the following statements concerning documentation (finding documentation, formats)?

There were 29 comments on other types of documentation that would be helpful; summarising the most common:

- **More worked examples that are applicable to real situations** (including for existing functions, workflows and scripts, what each does in plain English (overall comment that Matlab does this well), incorporating assumptions and approximations used, more technical details for expert users, beamline-specific documentation) [12 requests]
- **Improved user manuals for routine uses of the software** (including for plotting, determining orientation matrices from inelastic data, tutorials and manuals for data

reduction/visualisation/data analysis, video tutorials, quick start guides, saving data, plot inspection, overplotting and scaling, how to write an instrument definition file, more for iPython) [9 requests]
- **Document expected behaviour of algorithms** (including how they relate to workflow, including a higher priority to documenting data types, for ISIS SANS) [8 requests]
- **Ability to download online documentation** (including as part of local installation) [2 requests]
- **Searchable documentation by algorithm names** [2 requests]

See Appendix A.4 for a full summary of comments.

There were 30 additional comments on how else the documentation could be improved; summarising the most common:

- **Improved algorithm documentation** (including clearer descriptions, more use cases and examples, how to use functions, address disparity of detail across algorithms documentation, frequently used routines for individual instruments, better scripting documentation) [14 requests]
- **Better discovery of algorithms** (including searching by purpose - difficult to find algorithms unless you know the name, index page of algorithms by category such as facility, user, or application) [9 requests]
- **Better links between documentation** (including beyond programming jargon, for physics and chemistry, between overviews and concepts, working examples, details of specific algorithms and functions, clarity between GUI and command line aspects) [4 requests]
- **Involve scientists in preparation of documentation** (including for instrument-specific documentation) [3 requests]

See Appendix A.5 for a full summary of comments.

2.6 Software Learnability and Barriers for New Users

There were 30 comments on how the learning process could be improved; summarising the most common:

- **Clearer tutorials and worked examples** (including for basic processing and for different instruments and facilities, ensure examples can be easily copied/pasted and manipulated, how-to guides, reductions for iPython notebooks, comment that even greater value was during the ISIS neutron school 2016, where a number of workshops doing fitting procedures was done) [16 requests]
- **Provide video tutorials** [3 requests]
- **Consider running technique-specific courses** (including for going through particular analysis paths followed by users of one method, e.g. direct inelastic reduction and analysis) [3 requests]

- **Provide a printed startup document for new users** (including key commands explained, links to relevant tutorials and Mantid page before they arrive) [2 requests]

See Appendix A.6 for a full summary of comments.

2.7 Maintenance and Technical Support

Given the complex and sophisticated nature of Mantid and its operating environment, it's not surprising that all but one respondent indicated they have encountered problems (see Figure 16), although the greatest proportion reported this occurred only 'Occasionally'. When problems were encountered, help was needed only 'Occasionally' in the greatest proportion of cases, with a much lower proportion requiring help 'Most of the time'.

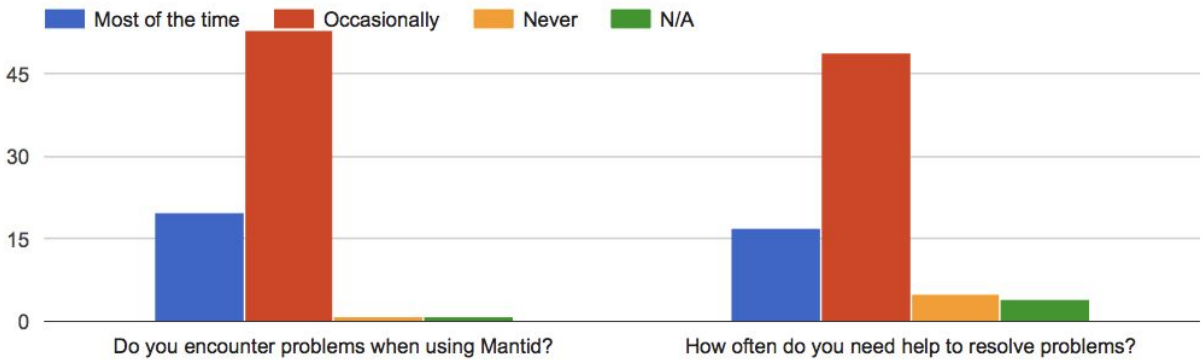

Figure 16. How often do you encounter problems when using Mantid, and how often do you need help to resolve them?

Generally, nearly half of the respondents indicated that the information made available to solve issues themselves was at least 'Ok' (see Figure 17), and nearly 20% indicated it was 'Good'. However, nearly 15% indicated the information was 'Poor'.

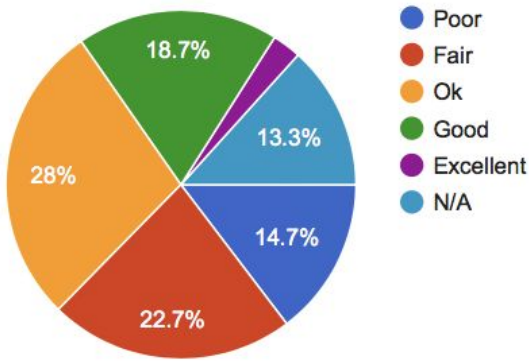

Figure 17. How would you rate the information made available to solve issues yourself?

In Figure 18, we observe that 30% of respondents indicated that they found the process of registering requests for new features and technical issues either very easy or quite easy (a significant proportion given that nearly 30% indicated that this was not applicable for them), with

nearly a third indicating this process was ok. However, 8.2% indicated this was a quite difficult process. None found it very difficult.

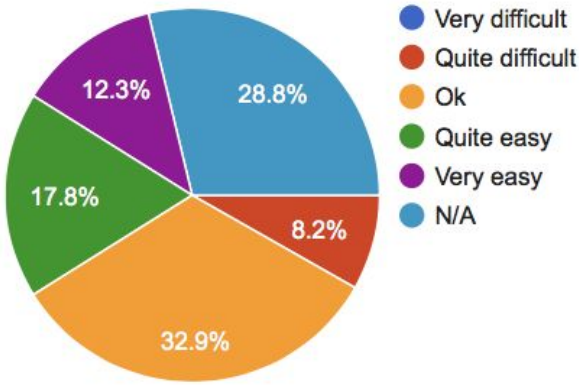

Figure 18. How difficult is it to register requests for new features and technical issues?

Half of the respondents indicated that the timeliness for incorporating technical fixes into releases was either good or excellent (see Figure 19), and the majority rated the timeliness for incorporation of new features generally good or fair.

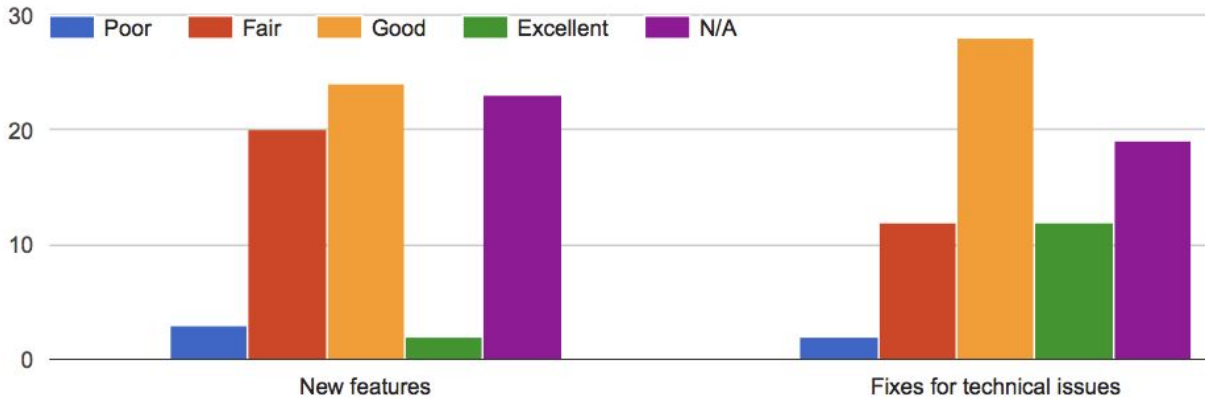

Figure 19. How would you rate the timeliness of delivering the following into future releases?

We also observe that the quality of fixing technical issues (see Figure 20) is generally ‘Good’ or ‘Excellent’ for a clear majority of those to whom that applies, whereas the balance of responses is clearly towards ‘Good’ for development of new features. The comparatively higher rating for quality of technical fixes over new features matches that observed for timeliness. The team is highly rated for their responses to general questions, with most responses indicating ‘Excellent’. The responses for solving problems using the software are centered around ‘Good’. In all these aspects, there are very few ‘Poor’ ratings, although a not insignificant amount of responses are ‘Fair’.

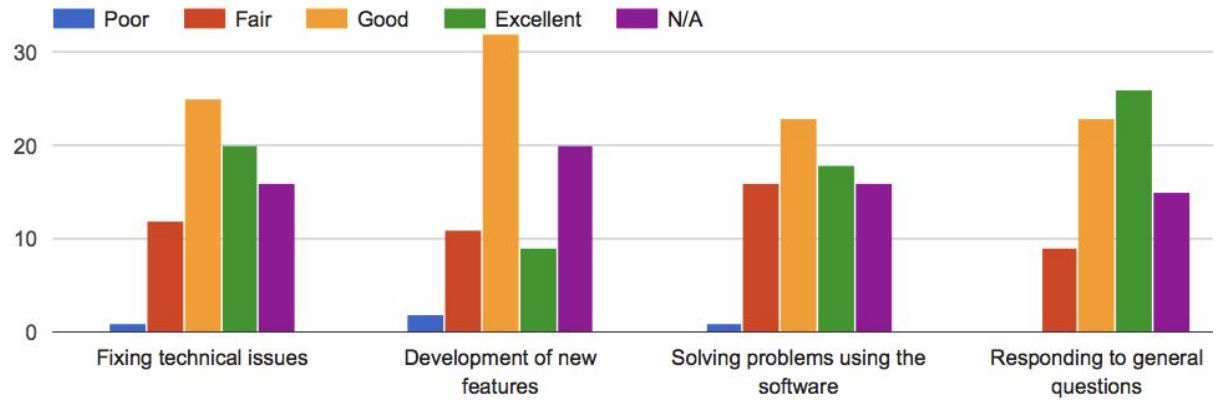

Figure 20. How would you rate the quality of support provided in the following areas?

In terms of the balance between providing new features and fixing bugs (see Figure 21), whilst the greatest number of respondents indicated the balance is 'Just right', there is a clear lean towards too much focus on new features, which is an interesting contrast considering the responses to timeliness and quality. This seems to indicate that fixing technical issues, whilst generally a more rapid and quality process, still needs comparatively greater attention and prioritisation compared to development of new features.

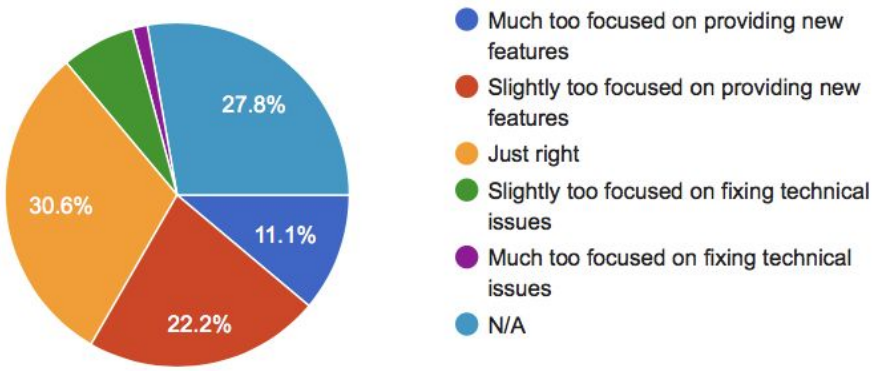

Figure 21. How would you rate the overall balance between providing new features and fixing bugs?

There were 17 comments on how support could be improved; summarising the most common:

- **Deliver support that is more technique specific** (including having an instrument specific technical expert within Mantid team (quality of support seems very much dependent on the instrument scientist), a need for science oriented or community specific help) [5 requests]
- **Address balance between fixing existing issues and new features** across the instruments (some indicate a greater focus show be on fixing issues, addressing quick fixes properly in the longer term, addressing general needs more quickly, in reflectometry there is an urgent need for both) [4 requests]
- **Provide other ways of resolving issues online** (in addition to on-site support, including a searchable database of a greater number of worked examples) [2 requests]

See Appendix A.7 for a full summary of comments.

2.8 Project Communication

In terms of using asynchronous methods of communication with the Mantid team, unsurprisingly 'Direct email' is clearly rated the most effective (see Figure 22). The 'User forum' and 'Mailing' list are both generally rated 'Good', although by far the greatest proportion do not use these methods. This may indicate an opportunity to promote these aspects of communication, perhaps developing a peer-based community of support, and would reduce the higher burden of effort on using email.

Figure 22. How would you rate the following for communicating with the Mantid team? (Asynchronous communication - user forum, mailing list and direct email)

For synchronous methods of communication, clearly 'Face to face' is most effective, as one may expect, and 'Telephone call' is generally effective where used (see Figure 23). Communication via Slack appears largely unused.

Figure 23. How would you rate the following for communicating with the Mantid team? (Synchronous communication - Slack, face to face and telephone call)

Whilst 'Face to face' is the communication method most highly rated, the preferred method is 'Direct email' (see Figure 24) by nearly half of respondents. It is interesting that the 'Mailing list' is not mentioned by anyone as a preferred method, although admittedly, it was comparatively rated the lowest of all communication methods.

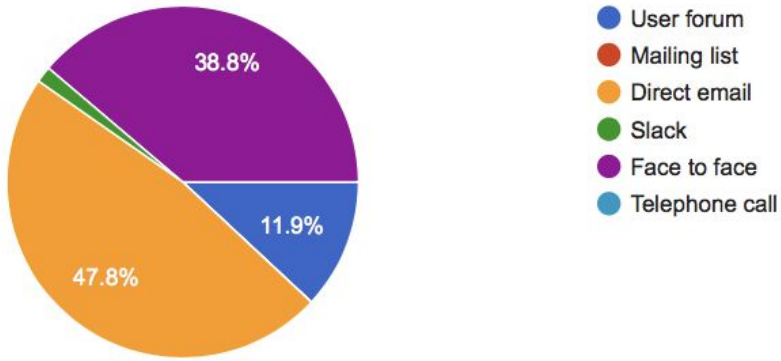

Figure x. What is your preferred method of interacting with the Mantid team?

The greatest proportion indicate they either 'Agree' or 'Strongly agree' that they are 'Sufficiently informed about what is happening with the Mantid project', although a not insignificant number of respondents 'Disagree' or 'Strongly disagree' with this statement.

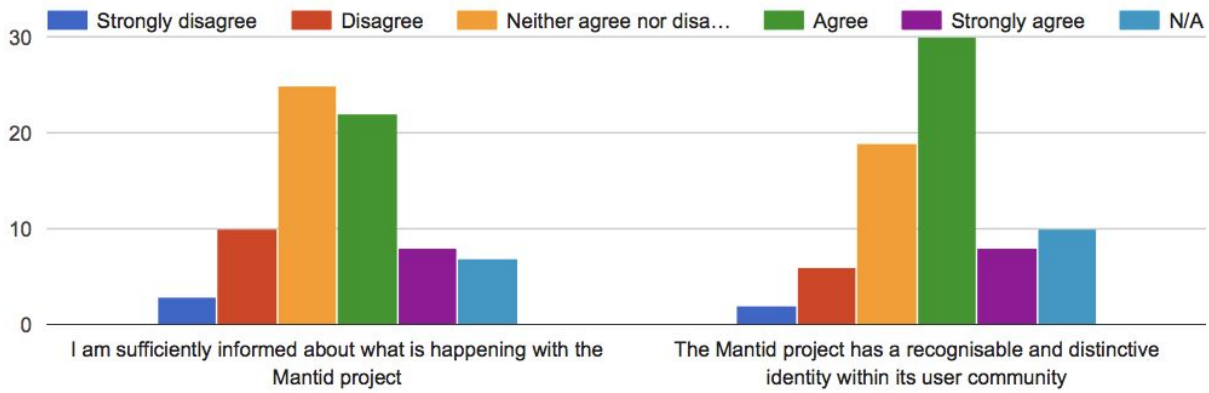

Figure 24. To what extent do you agree with the following statements (sufficiently informed and community identity)?

There were 18 comments on how communication could be improved; summarising the most common:

- **Greater level of communication about activities** (including use of newsletters, including users in communication not just instruments scientists, regular emails about updates targeted at specific instrument users) [4 requests]
- **Develop and present on the website a roadmap with timeline for planned developments for future releases** (including engaging the user and instrument scientist communities as a central part of the process) [3 requests]
- **Develop peer support community** (including promotion of and regular postings to the user forum, sharing algorithms) [3 requests]
- **More face to face activities with Mantid staff** (including presentations from Mantid, an annual user meeting) [2 requests]

See Appendix A.8 for a full summary of comments.

2.9 Training Events

45% of respondents indicated they have previously attended a training event for Mantid (see Figure 25).

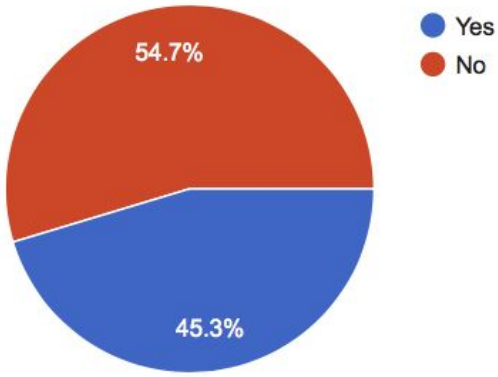

Figure 25. Have you attended a Mantid training event?

We can see from Figure 26 that 'Intermediate' training is most important to the clear majority of respondents, although 'Expert' and 'Novice' are also significantly represented.

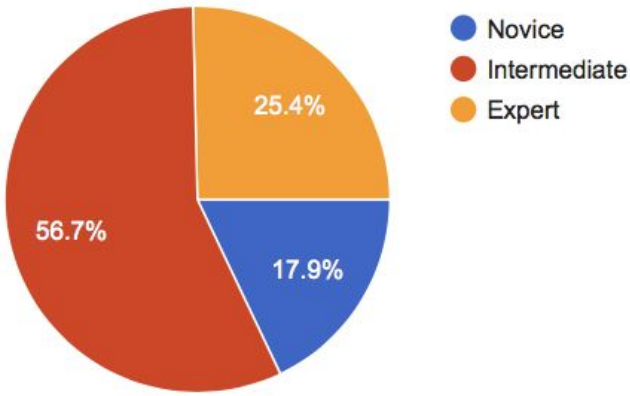

Figure 26. What level of training is most important to you?

Virtually all respondents that attended a training event (see Figure 27) indicated they either 'Agree' or 'Strongly agree' that it was clear what the event would cover and that it was useful in their work. All respondents either 'Agree' or 'Strongly agree' that that the event was well organised. Generally, respondents agreed that there are enough training events, and there was very strong agreement that the level of expertise available at their sites was adequate.

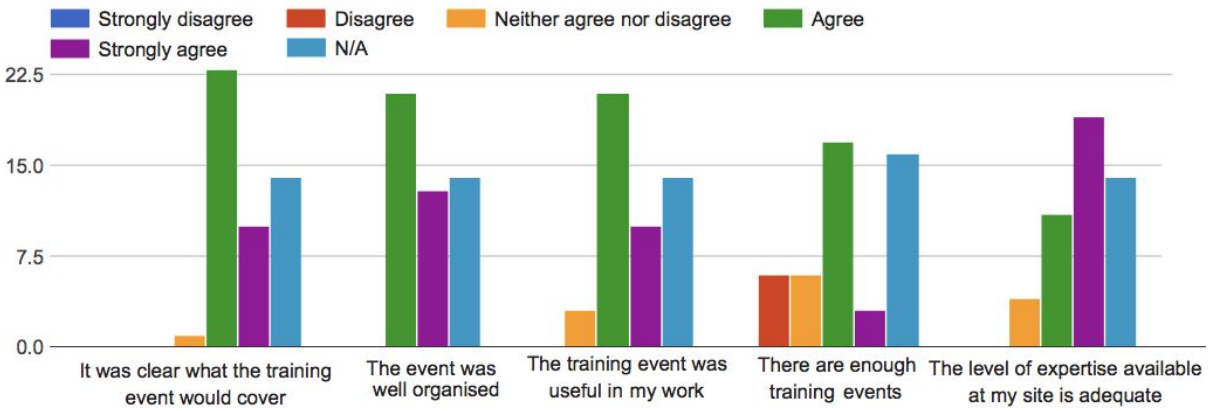

Figure 27. If you attended a training event, to what extent do you agree with the following statements?

There were 14 comments on types of training respondents would like to see organised; summarising the most common:

- **Science technique-specific training courses** (including for neutron scattering, direct geometry elastic, SANS) [5 requests]
- **A series of Python courses would be useful** (including object orientation, Mantid Python scripting) [3 requests]
- **Provide online tutorials** (including video tutorials, and see Matlab tutorials done by MIT) [2 requests]

See Appendix A.9 for a full summary of comments.

There were 15 comments on how else training could be improved; summarising the most common:

- **Provide training on specific scientific techniques** (including courses that introduce Mantid with more scientific depth, more specific to science groups e.g. powder diffraction) [3 requests]
- **More worked examples** (including through webinars) [2 requests]
- **Embed software engineers within experiments** [2 requests]
- **Regular user training events** (including generic (as we have now) and specific to techniques, perhaps presented as a satellite at the NWUM Meeting) [2 requests]
- **More documentation** (including e-learning courses for novices off-site) [2 requests]

See Appendix A.10 for a full summary of comments.

2.10 Project Governance

25% of respondents to date have attended a Scientific Steering Committee meeting (see Figure 28).

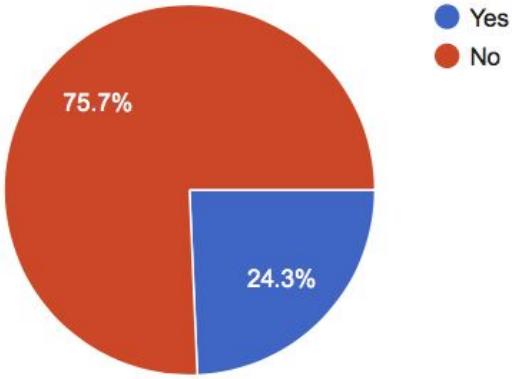

Figure 28. Have you attended a Scientific Steering Committee meeting?

There is very strong agreement that the project's activities are well aligned with its scientific objectives, and the project is generally able to make effective decisions (see Figure 29). However, there is a significant lack of knowledge concerning how the project is governed.

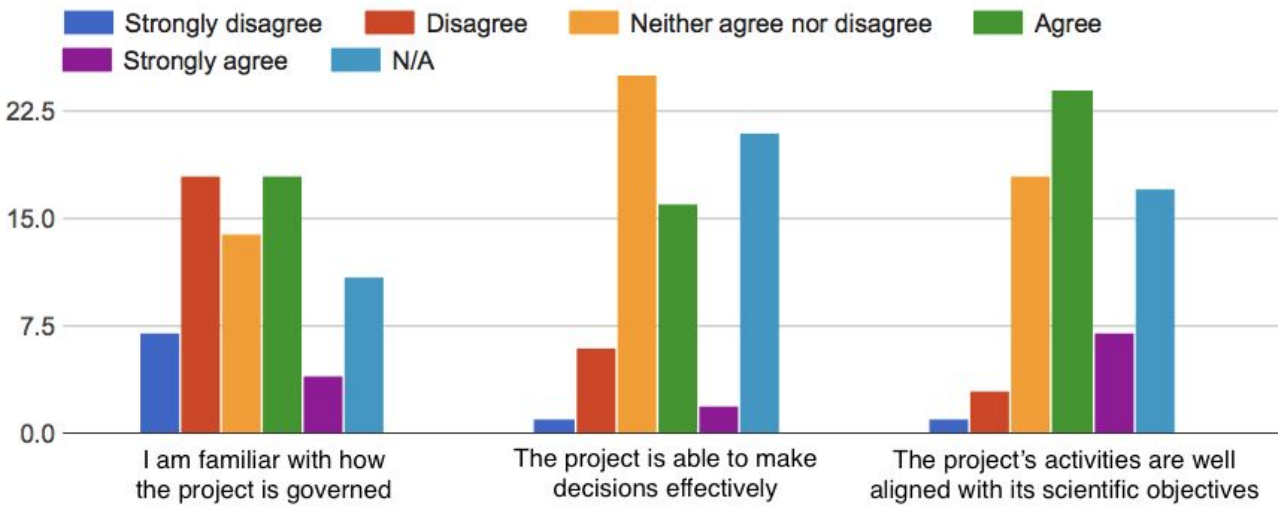

Figure 29. To what extent do you agree with the following statements? (Familiarity with governance, ability to make effective decisions, activities well aligned with scientific objectives)

Regarding whether there are enough resources and effort devoted to the project (see Figure 30), overall the respondents are neither showing strong agreement or disagreement. Whilst the greatest proportion of respondents are aware of how feature requests are generated and put into the development programme, a significant proportion are not.

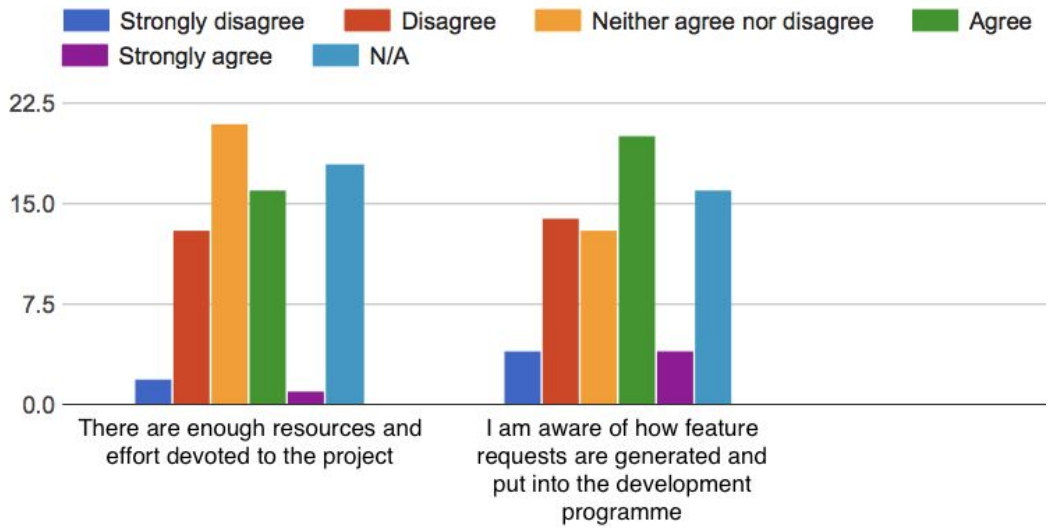

Figure 30. To what extent do you agree with the following statements? (Enough resources devoted to the project, awareness of how feature Requests are generated and put into development programme)

There were 18 comments on how governance could be improved; summarising the most common:

- **More communication with stakeholders** (including publishing meeting minutes, less filtering of SSC feedback to developers, need an explanation of how to submit requests, increase transparency on how things are decided, obtaining more input from front-line instrument scientists and users, provide open PMB meetings once a year, clearer communication of the project objectives in the short and medium term) [10 requests]
- **By trying to identify common features and synthesise communal solutions**, rather than duplicating or creating very similar algorithms [2 requests]

See Appendix A.11 for a full summary of comments.

2.11 General Comments

Due to the wide variety of the 14 general comments received, they are presented in their entirety:

- **Without Mantid and its continuing development my job would be impossible. It is incredibly challenging to deliver the level of complexity required and the team consistently deliver.** As I said previously, the main problems with the project probably lie with the organisation of the scientists who are feeding into it. Some suggestions from the Mantid team as to what sort of structures work would be good to see
- **The support at ISIS with regards to using this has been really good (particularly facilitated through WISH). The existence and support of NoMachine has also been really nice and we would not have been able to make progress without this.** My big concern is that there are basic functionalities that seem to be difficult in Mantid. These include basic plotting and also exporting data in a usable format. Thank you for the chance to comment on this. I hope this was helpful for you

- **In general I think the mantid project is very successful, and allows scientists to focus on the science and less the technicalities of how they get the data.** I believe having more resources devoted to the educating of users of the capabilities of mantid is the most important thing
- **The reflectometers have a lot of issues that need a concerted effort involving chasing scientists etc to get fixed**
- **Attempt to make Mantid more user friendly especially to new users**
- **Mantid is a fantastic tool, but you have to stay very current in its use to remember the many tricks of the trade!**
- **My experience with data reduction and processing has improved significantly over the last 5 years. Much of that results from the streamlining of reduction with MANTID.** I think there is still more to be done, esp. for visualization, and it would be great if this could happen at a faster pace (more people working on this!) and with the input of users about what we need. I still use DAVE for most of my post-reduction visualization.
- **Some instruments use more than one technique which can have very different take on the survey**
- **I couldn't give much input related to the communication, support and governance of Mantid as I haven't been exposed to those aspects**. I have mainly used Mantid for basic data reduction during or soon after experiments
- **If an alternate to Mantid exists or can be developed for SANS reduction, it might be better given the memory and speed issue**
- **Mantid has made great progress but it would be highly useful to have a configurable "tool box" like layout** that would in an intuitive fashion enable users to create an environment specific for a technique or scientific problem and not take long waiting time to load a file, crash when displaying a file in 3D, or simply not finding the right algorithm in the list because the user cannot remember the word to start with. A better sorting of algorithms and adjustable, robust startup workflows for specific techniques would help. A large disadvantage is that nothing is real time, loading of data sets takes many minutes (even for small files). Real time, interactive visualization with feedback to Mantid would make this software really useable and useful. Interactive would not be zooming in and out but integration of 3D peaks, background fitting, peak development with measurement time
- In fastgr, after messing around with Q min, Q max, r max, etc, and generating and comparing PDFs, **I would like the "save PDF" button to give me a properly formatted PDF with the appropriate headers, instead of the simple format it currently outputs**
- **Thanks for your work and support!**
- **Thank you very much for Mantid**. If you can solve the little bug I mentioned before that could be great

Appendix A - Record of Comments Analysis

A.1 How could data reduction be improved?

Comment	Count
Data processing and access speed should be improved, in some cases significantly (on the fly analysis, reduction, perhaps take advantage of event based data for better speed and accuracy of representations of the data, speed on legacy instruments)	13
Better documentation and support for new users (user scripts should have an easy manual for new users, better docs on reduction options e.g for SANS)	6
Improve resilience against crashes	4
More user-friendly (data plotting e.g. work on MSLICE for data plotting will improve things, good starting values and simple interfaces to change the settings need to be added (for plotting multidimensional spaces), plotting needs to be simplified in the respect that zooming and reading of datapoints needs to be improved)	4
Improved corrections (for multiple scattering and absorption)	3
GUI interface that works across all direct geometry instruments (removing need for custom scripts for each instrument)	3
Further automation for reduction (for non-ISIS instruments, routines specific for VESUVIO should be added)	2
Improved tracking of run meta-data	1
Where graphs appear should be better organised	1
Exporting data in a format that can be easily plotted and manipulated in other programs	1
Ability to reprocess data at home outside of the beamline script	1
Stitching of datasets could be improved, in terms of capability and accuracy	1
Access to real time data	1
Minimizing the size of user-defined mask files that are generated by the mask-drawing tool in the SANS interface	1
Utilize metadata to identify transmission runs, scattering runs and suggest relations between a scattering run's associated transmission	1
For single crystal data, a more intelligent slice viewer would be beneficial	1
More control over parameters so that one can remove faulty detectors from reduction script	1
Better integration with instrument control and with analysis programs	1
Perform more reduction in-place, without allocating more resources to completely copy the workspace.	1
Would be useful to be able to generate I(Q) vs phi plots in Mantid (though this can be done e.g. using SASview)	1
Being able to visualise I(Q) vs Q live as the sample scatters	1
Make the "final reduction" more open (involve users in the "final choices" of this process with streamlined and step-by-step final reduction scripts)	1

Maintain backwards compatibility	1
Plotting quality (for publications)	1
Improved handling of multiple groups of detectors within the same dataset.	1
the MANTID GUI is often slow and the visualization tools are extensive but not intuitive	1

A.2 Which barriers prevent better integration between Mantid and your working processes?

Comment	Count
Reliability (including when processing single crystal data, while using some of its algorithms in scripts to post process data, unwillingness to give Mantid to external users due to instability, reliability on Mac, copy/pasting into tables seems to give random results, need for robust fitting routines)	9
Lack of user manuals (including for inelastic neutron scattering with time-of-flight direct geometry instruments, basic tasks, code examples, for plotting)	6
Data plotting and visualisation within Mantid (including plotting of direct geometry is not done via Mantid (it is noted that an improved version of MSLICE integrated into Mantid is in the works), difficult to learn, not able to produce Matplotlib figures within Mantid)	6
Data reduction takes a long time (even for a single data set, suggest having a dedicated cluster for every instrument in the beam line, faster so reduced data can be produced and analysed fast enough to influence decisions on the beamline)	5
The occasional bugs which arise due to changed requirements for inputs to algorithms which break reduction scripts (algorithms change from one version to another (keywords are suddenly required and nobody knows what they are supposed to mean))	4
Need more fundamental algorithms incorporated into Mantid (e.g. adsorption corrections, multiple scattering corrections, transformation to phonon density-of-states; better access to fitting algorithms with resolution effect incorporated)	3
Exporting data in a timely and helpful format (including for use in Matlab, Fullprof (GEM and WISH), Inability to output data in .nxs format directly from the workspace (for WISH), use with simulation software)	3
Mantid too complex (including the production of reproducible publication quality plots is too complicated)	3
How Mantid deals with displaying windows (it resets a lot of windows every time a data file is loaded, difficult to find certain windows)	2
Lack of full implementation of Horace style command line interface and functionality	1
The use of specialised powder refinement software	1
More automation and choice of integration method for single crystal	1
Perhaps have MATLAB and other languages code available to splice and analyse data	1
background and/or normalization fits often not sufficient quality	1
The data merging needs to be improved, needs more funtionalites on 2D q space data.	1

The fact that I need to log into the cluster to use it	1
Biggest barrier is having to use nomachine for large data sets. Not sure there is any way around this though. Is there a version for installation on Ubuntu?	1
The absence of pipeline functionality before and after Mantid	1
Integration of self-prepared scripts with a structure that I cannot modify [lack of customised use of scripts]	1
I often find myself doing a large amount of data reduction and analysis on mantid, to then export it all to text files and plot in pure python.	1
new measurement methods at ISIS (Time Resolved Prompt Gamma) which we would like to have integrated in the Mantid suite, together with data repository (ISIS Catalog)	1
More extended features in the VESUVIO data reduction require development of additional scripts/algorithms	1
Version control needs to be improved - every day I open Mantid I am wondering if if will be the same Mantid as yesterday or which instrument definitions or procedures may have changed	1
Have had trouble examining and reducing data from ILL with mantid software.	1
Transparency in what algorithms are being applied and what operations are doing done in IDL vs Mantid	1
Would be nice to dispense with the graphical interface completely and just incorporate this into my python code	1
Data structure within .h5 produced by Mantid	1

A.3 What would you like to see improved in the software?

Comment	**Count**
Improved stability (including improvement of system tests, reduction, MantidPlot, random crashes, better memory management for reliability, resolving bugs for table copy and paste, Mac stability)	18
Improved data plotting (including simpler plotting, 3D plotting, easier integration of 2D/waterfall/3D plots, better quality figures for publication, line zooming is awkward, options of inspecting the plot need to be direct access of options for inspecting plots via shortcuts)	12
Improve ease of use (including cleaner GUI interface for specific applications, a simpler command set, less reliance on GUI, universal GUI for direct geometry instruments, easier modifying of algorithms, easier visualisation of algorithm tree index)	7
Improved processing speed (including SANS reduction, Catalog when selecting multiple files)	5
Better fitting (multi-peak, full pattern, pole figures, handling multiple datasets, background fitting)	4
Improved export capabilities (for graphics, data, 2D maps from batch reduction (ISIS SANS), compatibility with fullprof)	3

Better documentation (including a user manual for scripting and built-in features, guide to setting up an instrument via instrument definition files, more contextual help)	3
Improved saving of projects (including having previous settings and saved plots return when reloaded)	2
Better integration with the iPython notebook	2
Improved installation	1
Better and less frequent updates	1
Easier use for single crystal integration	1
Better communication on things like calibrations of instruments across facilities	1
Automatic synchronisation between instrument drive and local PC	1
Batch reduction (ISIS SANS)	1
Azimuthal scans with varying bin sizes for SANS data	1
Improved masking on SNAP	1
More automation	1
Ability to set number of environments (different profiles on top of instruments to start various algorithms and load workspaces)	1
Improved error handling in scripts (indicating a property is missing rather than providing a generic error, etc)	1
Resolving issues with beamline instrument definition files	1
Improved reflectometry reduction scripts	1
A faster release of pre-compiled updates for newer linux distributions	1
When create a new blank form, it always read-only and need to be double click and change the property.	1

A.4 What other types of documentation would be helpful?

Comment	Count
More worked examples that are applicable to real situations (including for existing functions, workflows and scripts, what each does in plain English (overall comment that Matlab does this well), incorporating assumptions and approximations used, more technical details for expert users, beamline-specific documentation)	12
Improved user manuals for routine uses of the software (including for plotting, determining orientation matrices from inelastic data, tutorials and manuals for data reduction/visualisation/data analysis, video tutorials, quick start guides, saving data, plot inspection, overplotting and scaling, how to write an instrument definition file, more for iPython)	9
Document expected behaviour of algorithms (including how they relate to workflow, including a higher priority to documenting data types, for ISIS SANS)	8
Ability to download online documentation (including as part of local installation)	2
Searchable documentation by algorithm names	2

Online database of frequently asked questions and answers (like Matlab)	1

A.5 How else could the documentation be improved?

Comment	Count
Improved algorithm documentation (including clearer descriptions, more use cases and examples, how to use functions, address disparity of detail across algorithms documentation, frequently used routines for individual instruments, better scripting documentation)	14
Better discovery of algorithms (including searching by purpose - difficult to find algorithms unless you know the name, index page of algorithms by category such as facility, user, or application)	9
Better links between documentation (including beyond programming jargon, for physics and chemistry, between overviews and concepts, working examples, details of specific algorithms and functions, clarity between GUI and command line aspects)	4
Involve scientists in preparation of documentation (including for instrument-specific documentation)	3
Better plotting documentation (including for Jupyter Notebooks to understand how data is output)	1
More information about fundamental data treatment, specifically for event based data manipulations	1

A.6 How could the learning process be improved?

Comment	Count
Clearer tutorials and worked examples (including for basic processing and for different instruments and facilities, ensure examples can be easily copied/pasted and manipulated, how-to guides, reductions for iPython notebooks, comment that even greater value was during the ISIS neutron school 2016, where a number of workshops doing fitting procedures was done)	16
Provide video tutorials	3
Consider running technique-specific courses (including for going through particular analysis paths followed by users of one method, e.g. direct inelastic reduction and analysis)	3
Provide a printed startup document for new users (including key commands explained, links to relevant tutorials and Mantid page before they arrive)	2
Improve algorithms (including clean algorithm list, standardise names, remove duplicate algorithms)	1
Very technical aspects such as defining a new instrument and testing are extremely challenging	1
Improved GUI (including less on the main page)	1
Embed Mantid software engineers to train instrument scientists during experiments	1
Separate Mantid apps which hide the complexity	1

Organise workshops on Mantid when beamline is off	1
Provide clear descriptions on the various objects populated by data (e.g. how MD differs from a workspace)	1
Have an online discussion forum	1
Muon e-Learning course helped considerable during recently Muon School; consider whether this type of learning could be extended	1
Occasional emails targeted to instrument-specific users about new features and links to documentation on how to use them.	1

A.7 How would you like to see support improved?

Comment	Count
Deliver support that is more technique specific (including having an instrument specific technical expert within Mantid team (quality of support seems very much dependent on the instrument scientist), a need for science oriented or community specific help)	5
Address balance between fixing existing issues and new features across the instruments (some indicate a greater focus on issues, addressing quick fixes properly in the longer term, addressing general needs more quickly, in reflectometry there is an urgent need for both)	4
Provide other ways of resolving issues online (in addition to on-site support, including a searchable database of a greater number of worked examples)	2
Develop a framework describing how scientists should work together (probably it is the scientists who need to be better organised, not the Mantid team)	1
Focus on fundamental aspects such as plotting and exporting data in usable formats	1
A cleaner Mantid architecture would greatly reduce effort in identifying and resolving issues	1
Mantid is difficult to work with because the language used in algorithms or the help menus is not general and not intuitive to most scientific communities if they are not programmers	1
Clearer indication of lines of responsibility for support	1

A.8 How would you like to see communication improved?

Comment	Count
Greater level of communication about activities (including use of newsletters, including users in communication not just instruments scientists, regular emails about updates targeted at specific instrument users)	4
Develop and present on the website a roadmap with timeline for planned developments for future releases (including engaging the user and instrument scientist communities as a central part of the process)	3
Develop peer support community (including promotion of and regular postings to the user forum, sharing algorithms)	3

More face to face activities with Mantid staff (including presentations from Mantid, an annual user meeting)	2
Investigate using Slack as a way to improve discussions with the user community	1
Clarify who is responsible for each aspect of the codebase, to expedite communication	1
Often people can miss out on new features or existing solutions to their problems, due to other commitments or lack of general interest in finding out	1
An automated report on crashes could be useful	1
Develop a list of frequently asked questions and answers	1

A.9 Is there any type of training that you would like to see organised in the future?

Comment	Count
Science technique specific training courses (including for neutron scattering, direct geometry elastic, SANS)	5
A series of Python courses would be useful (including object orientation, Mantid Python scripting)	3
Provide online tutorials (including video tutorials, and see Matlab tutorials done by MIT)	2
Provide training on instrument definition files	1
Providing training to general users (perhaps linking the training notes and data from the instrument websites)	1
Training on finding the UB matrix, autoreducing the data, plotting and data analysis	1

A.10 How could training be improved in the future?

Comment	Count
Provide training on specific scientific techniques (including courses that introduce Mantid with more scientific depth, more specific to science groups e.g. powder diffraction)	3
More worked examples (including through webinars)	2
Embedded software engineers on experiments	2
Regular user training events (including generic (as we have now) and specific to techniques, perhaps presented as a satellite at the NWUM Meeting)	2
More documentation (including e-learning courses for novices off-site)	2
If training is an option for PhD students using this software it could be useful	1
I was not aware training was a possibility	1
All levels of training are important for different aspects of science. Mantid is intended to be a neutron data processing and analysis platform not a programming compendium. It should be managed as such.	1

A.11 How do you think the governance could be improved?

Comment	Count
More communication with stakeholders (including publishing meeting minutes, less filtering of SSC feedback - developers should hear more directly, an explanation of how to submit requests, transparency on how things are decided, obtaining more input from front-line instrument scientists and users, open PMB meetings once a year, clearer communication of the project objectives in the short and medium term)	10
By trying to identify common features and synthesise communal solutions, rather than duplicating or creating very similar algorithms	2
Remove two tier membership(to avoid non-partner specific implementations)	1
Strong leadership of the Scientific Steering Committee	1
Scientific Steering Committee representatives should ensure wider consultation forms the basis of their representation, and not personal opinion (based on specific areas upon which to obtain feedback, filling out detailed questionnaires in advance)	1
Intermediate (6-monthly) facility-level SSC meetings (with well defined go-to people on each scientific area but also others (on a rota) that are not necessarily fully engaged with Mantid to ensure their views are represented	1