Minutes of the Endurance PMC meeting

BASTILLE

Monday, 13 March 2017, at 10:00 a.m. in the seminar meeting room

Present: Ian Bush, Franck Cecillon, Charles Dewhurst, Dirk Honecker, Bela Farago, Emmanuel Farhi, M. Teresa Fernández-Díaz, Miguel A. González, Mark Johnson, Paolo Mutti, Xavier Philippe, Lionel Porcar, Sylvain Prevost, Verena Reimund, Helmut Schober, Charles Simon, Antti Soininen, Gagik Vardanyan.

Excused: Gabriel Cuello, Björn Fåk, Giovanna Fragneto, Thomas Hansen, Eric Pellegrini, Thomas Saerbeck, Tilo Seydel.

Agenda:

- Update on project status and progress
- Project plan for 2017
- Staff matters: Prolongation of I. Bush's contract
- Discussion

C. Simon chaired the meeting. M. A. González (MAG) started it with a presentation of the current status of the project, the evolution since last PMC meeting on November 3rd 2016 and the plans for 2017. The presentation is available at: http://intranet.ill.eu/divisions/dpt/millennium-endurance-programmes/phase-m-2/pmc-meetings/2017/bastille-130317/
Discussion took place during the presentation.

MAG explained that since last PMC meeting, Mantid has been deployed on IN16B and users have been able to try it during the first cycle of 2017 (19/01/2017 to 08/03/2017). No major problems have been reported by Tilo Seydel (instrument responsible and backscattering contact person for Mantid) and the work done at ILL has been included in the last general Mantid release done in February (version 3.9). Users can use a single graphical user interface (GUI) or write a script. M. T. Fernández-Díaz enquired if such scripts could be created automatically and MAG replied that they can be created very easily from a button in the GUI. H. Schober asked about the future TOF option in IN16B (BATS project). MAG replied that there have been some discussions with Tilo Seydel about this and other possible changes in IN16B, but that no work can be done until the project is more advanced and the new requirements can be specified.

Concerning TOF instruments, IN5 has been added so now Mantid can be used for IN4, IN5 and IN6. And the reduction workflow has been split into chunks. First tests look positive and the next steps are to create a spreadsheet interface and get further user feedback. A small meeting with the TOF instrument responsibles will be organized on March 31st with this purpose. B. Farago asked in which language are the interfaces written. There is not a single answer. The IN16B interface is written in C++, TOF interfaces are self-generated, and the future spreadsheet interface will be written in Python. H. Schober asked if he could do everything that he was used to do with Lamp. MAG answered that Mantid will provide at least the same functionality, although some tools will not be completely equivalent and will require some adaption from part of the user, in particular in what refers to plotting. H. Schober asked which is the expected performance when treating single crystal experiments in IN5. MAG answered that this has not been tested yet and that single crystal work is not included in the ILL

project, so we will rely on the developments done at ISIS. It was recognized that the large data size of IN5 files imposes some fundamental limits. But the actual treatment already involves managing large data sets because the data are not collapsed into constant 2θ bins, and the times needed to correct the data are reasonable (of the order of 1-2 minutes per data set).

For reflectometry, loaders for D17 and Figaro have been written and the team is exploring the different approaches developed at ISIS and SNS and how they can be adapted to ILL necessities. The aim is to provide a reduction workflow with a 'Cosmos-like' GUI by December 2017.

For powder diffraction, loaders for D1B and D20 exist, as well as the instrument definition files for D2B and D4C. The purpose is to cover the basic needs of D1B and D20 by June 2017.

A new task has been incorporated into the project, related to the development of a new Mantid workbench breaking some backwards compatibility (Mantid v. 4). This decision was taken by the steering committee of the Mantid project and the ILL requested to contribute as a partner member. H. Schober asked if the ILL is a fully-fledged member of the collaboration. M. Johnson answered affirmatively, although the official documents have not yet been signed and send to ISIS.

Action: M. Johnson will send the documents to P. Mutti, who will replace him in the Mantid steering committee.

B. Farago asked which would be the effects of breaking the backwards compatibility. I. Bush answered that probably some existing scripts would not work in Mantid 4. In the past, ISIS helped their users to update the scripts when similar changes happened. B. Farago asked which was the contribution of the other facilities to Mantid 4. I. Bush answered that both ISIS and SNS will dedicate two persons each for one year, and ESS and ILL one person each for half a year.

The ILL team is also contributing to the development of the new instrument geometry (Instrument 2.0) in Mantid, which is an activity lead by ESS. As it has been decided that this new instrument geometry offers a more flexible and performant framework to implement the scanning instruments, I. Bush has started to collaborate with other members of the Mantid collaboration in its design and will then use the new geometry to implement the ILL scanning instruments. This should be completed before July 2017. B. Farago asked who the main contributor to this activity was. I. Bush answered that it was the ESS, but that ILL was interested in contributing to implement early some parts for the benefit of the work related to the scanning instruments.

Work on SANS will start after the summer. The reference software used as a benchmark for the necessities of ILL scientists and users are Grasp and Lamp. Additional discussions with the SANS scientists will take place, particularly to determine possible issues when handling big data sets, as some concerns in this sense have been raised by S. Prevost based on past experiences with Mantid at ISIS. H. Schober asked if polarization analysis was handled by Mantid. MAG answered that we had not look at this, but that Polref at ISIS is treated by Mantid, so this is not expected to be a problem. At the ILL it is planned to treat D7 with Mantid, but the work will be initiated only once the work on the general techniques is done.

I. Bush contract will be extended for a second year. This is needed in order to account for the extra effort needed for Mantid 4 and to keep a team of developers of reasonable size during 2017, as V. Reimund will leave on maternity leave and the reduced size of the CS group does not allow any additional contribution from it.

A new high-level Gantt chart was presented. B. Farago asked if TAS instruments will be included. MAG answered that not in the current project. P. Mutti added that he has had some contacts with TAS scientists in order to look for long-term solutions for TAS software. C. Simon asked which other instruments are not included in the Mantid project. The answer is NPP instruments (SCI provides

support to them outside Mantid) and single crystal diffractometers (supported by an ongoing separate project – NSXtool). The division between CS activities and the project is now made clear in the new project plan and it was clarified that the Phase I of Bastille is focused only on data reduction using Mantid.

C. Simon asked about scanning in SANS, e.g. in vortex studies. M. Johnson clarified that the notation 'scanning instrument' is being used in the project to refer to instruments with moving detectors, where several acquisitions need to be combined and merged into a single workspace. Other types of scans, such as sample rotations (e.g. omega-scans) or motor scans (e.g. rocking curves), which do not imply a detector motion do not pose a problem in Mantid.

H. Schober asked about support for data reduction during the project execution. M. Johnson indicated that a transition period is needed. MAG added that this is outside the project, but that Lamp is still used and supported, although no large new developments will be done in Lamp.

M. T. Fernández-Díaz asked when the work for D2B will be completed. MAG answered that the current plan is that by the end of June 2017 the independent work done on the implementation of the scanning instruments and the data treatment for D1B/D20 is done and can be combined to deal with D2B by the end of September 2017.

H. Schober asked if there are changes in the scope in the new project plan. MAG answered that only the additional effort for Mantid v. 4 has been added, but that the scope has not changed.

H. Schober asked about the risk analysis. MAG said that the initial risk analysis is maintained, although a new risk has been added in order to account for the need of maintaining and supporting Mantid adequately after the end of the project. Some discussion ensued about possible difficulties if Mantid is not delivered on time or supported afterwards, as well as about contingency plans to support Lamp and other needed software. It was agreed that this is outside the scope of the project and that future solutions should be discussed between the management, SCI and CS.

A point emerging from the discussion was how to deal with old data, as the treatment of data collected before the project's start is not actually foreseen. Existing software should be maintained accessible for as long as is needed, but C. Simon and H. Schober asked Mantid to be able also to treat the data collected during the last 5 years. P. Mutti said that converting data stored with the old ASCII format to the new NeXus format is straightforward (SCI has already appropriate translators), so this is not an issue for instruments that have not changed in this period. In cases where the instrument has been modified or upgrade, the situation is more complex and this new request will have to be examined case by case.

S. Prevost said that the Mantid project is now 10 years old and he asked what this represented in terms of the maturity of the framework. I. Bush replied that many parts of the framework are mature and work well, but that new requirements appear constantly bringing new needs for large refactoring tasks. M. Johnson added that ISIS and SNS have always been aware of the continuous effort required to ensure Mantid works well and they put the needed resources to achieve this.

C. Simon thanked all participants and closed the meeting.