Agenda and Minutes

Workshop III WP10

Wednesday 6th June 2018

Opening

14:30 – 14:35	Local organiser	Joachim Wuttke
14:35 – 14:40	Program committee	Joachim Wuttke
14:40 – 15:00	Chairman	Thomas Holm Rod

SINE2020 Projects SasView, BornAgain

| 15:00 – 15:40 | Agile methodology, GUI testing and SasView status | Piotr Rozyczko |
| 15:40 – 16:10 | BornAgain status | Walter VanHerck Dmitry Yurov |

Projects outside SINE2020

| 16:40 – 17:00 | NSXTool | Jonathan Fisher |

SINE2020 Project Mantid

17:00 – 17:10	Mantid at ILL	Miguel Gonzalez
17:10 – 17:20	Scanning instruments in Mantid	Vardanyan
17:20 – 17:35	Mantid at MLZ, MD workspace	Marina Ganeva
17:35 – 17:45	Mantid at PSI	Emmanouela Rantsiou
17:45 – 18:00	TOF quick visualisation in Mantid	Soininen

Thursday 7th June 2018

SINE2020 Project QENS

9:00 – 9:20	Reverse fitting in spectroscope	Jakob Lass
9:20 – 9:40	QENS model library and jupyer notebooks	Celine Durniak
9:40 – 9:55	Ab-initio and other INS QENS analyses in Mantid	Sanghamitra Mukhopadhyay
9:55 – 10:10	QENS alayses in Mantid	Hewer

SINE2020 Project Imaging

| 10:10 – 10:25 | Tomographic reconstruction with Mantid Imaging | Daniel Nixon |
| 10:25 – 10:45 | Corrections in imaging and project status | Anders Kaestner Chiara Carminati |

SINE2020 Project µSR

| 16:30 – 16:40 | Workflow for µSR analysis | Bonfa |
| 16:40 – 17:00 | Simulation and refinement for µSR | Onuorah |

Standards and technology – Formats

| 17:00 – 17:15 | Geometry in NeXus | Matthew Jones |
| 17:15 – 17:30 | Scanning data in NeXus | Tobias Richter |

Standards and technology – GUI

17:45 – 18:00	Lessons from User Experience Course	Wojciech Potrzebowski
18:00 – 18:40	GUI for BornAgain	Gennady Pospelov
18:40 – 19:00	Testing GUI an disentangling signalling spaghetti	Joachim Wuttke

Friday 8th June 2018

Standards and Technology

| 9:00 – 9:30 | Fit benchmarking Python library | Anthony Lim |

SINE2020 Project MDANSE

| 9:30 – 9:45 | MDANSE | Remi Perenon |

Projects outside SINE2020

| 9:45 – 10:00 | Quantum Materials studies using BIFROST@ESS | Johan Hellsvik |
| 10:00 – 10:15 | SpinW | Simon Ward |

Standards and technology – Documentation

| 10:45 – 11:10 | Online documentation | Gennady Pospelov |
| 11:10 – 11:35 | Producing tutorial videos | Anders Kaestner |

Standards and technology – Outlook

| 11:35 – 12:05 | Tensorflow | Jonathan Fisher |

Discussions

Topic	Owner
SasView & BornAgain	Wojciech Potrzebowski
Imaging & data formats	Anders Kaestner
INS	Simon Ward
QENS	Celine Durniak
muon	Anthony Lim
Packaging	Marina Ganeva
Mantid	?
Materials libraries	Gennady Pospelov
Final WP10 deliverables	Thomas Holm Rod

SasView & BornAgain (Wojciech Potrzebowski)

Topics covered:

1. Scatter program

2. Engagement of external stockholders into SasView and BornAgain

3. Combined SasView-BornAgain code camp

Ad. 1. There is a particular interest in incorporating Scatter program into BornAgain or possibly SasView. These efforts can and should be coordinated between SasView and BornAgan development teams. There are some functionalities that can be relatively easy to implement in SasView while the others are easier achievable from BornAgain. The development of beta-approximation within SasView framework that is planned for coming months should reduce workload for Scatter integration. Wherever possible Scatter models should be readable both for SasView and BornAgain and ideally should be located in the common library.

Ad. 2. The engagement of external stakeholders was discussed. One possible way for engaging developers from SasView and BornAgain team is to involve them in the review process (particularly for major releases) and participate in Demo sessions. Once this approach settles down and proves to work fine it be extended to other stakeholders (e.g. instrument teams). BornAgain version 1.12 should be already exposed to instrument teams.

Ad. 3. The idea of having joined SasView-BornAgain code camp was discussed. Due to busy calendars this is not possible this year but it hasn't been ruled out for future.

Imaging (Anders Kaestner)

INS (Simon Ward)

- 8 participants attended, coming from ESS, PSI, Nordita, ILL, MLZ and ISIS
- 2 people present had practical experience with INS
- We had a discussion on peoples experiences and expertise.
- This lead to a discussions on the state of Mantid and future data processing.
- We also discussed experimental practicalities
- This lead to the discussion on why MATLAB based solutions are currently preferred.

QENS (Celine Durniak)

QENS discussion - SINE2020 WP 10 - Thursday May 7th 10h45

Attendees: about 10 persons (Nordita, DMSC ESS, ILL, MLZ, ISIS)

Summary:

During this session, a brief description and updates of the tools related to the treatment of QENS data were given, focusing on the status and possible developments of the QENS models library, the features to be released in the new version of Mantid, and two projects at SNS: QClimax and qef. Testing of some of the new developments (library and fitting in Mantid) will follow-up in the near future.

Details

QENS model library

- it was emphasised that it was not only meant for Mantid.

Anders gave a more thorough description of the problem in Mantid to use Python script and user defined function

- Some of the macros in Dave would be useful to have in the library

The status of two SNS projects was briefly discussed

- Climax from Timmy: it is to be used remotely only via script (no GUI) and it is not open source.
- qef from Jose Borreguero was compared to our library. The former contains more than models.

The question of its status as an SNS project or as a personal development was raised.

Then we talked about the new developments in Mantid:

- global ties for fitting will be available in the next release
- it is/will be possible to load data in the interface (not restricted to ISIS instruments anymore)
- Mantid already has jupyter / ipython notebooks

Ideas mentioned:

- (long term): fit raw data not reduced (S(q, E or omega)).
- generate notebook from Mantid's GUI

Decisions:

- The scientific computing group could involve some resources to QENS if agreed with ESS in-kind contributions.

- J. Wuttke will test the QENS model library and provide feedback.

- Sanghamitra will ask a few of the attendees to test new QENS features in Mantid.

- The next step for the QENS library will be to add examples using one of the minimisers in Mantid and a way to add the background.

Muons (Anthony Lim)

As for the muon discussion group, it was fairly brief. We talked about the next steps. Since the project has completed the goals set out in SINE2020 Roberto reported back that he has requested to be allowed to extend the MUSR code. Other than that we discussed general muon problems.

Packaging (Marina Ganeva)

Report from the packaging discussion

- about 10 participants

- none of the participants has experience with the public repositories

The requirements to the software installation routine:
- should be easy for unexperienced user
- should be easy to automatise for installation on many computers (for example, across the facility)

Python software
- the easy way is to distribute is to write a script for pip (MJOLNIR)
- the installation in the case is done just with pip install and meets both requirements

C++ software
Win/Mac:
- the best way is to create an all-in-one package, which contains all the dependencies (sometimes even a Python with libraries)
- this package will work, the problem of unmet dependencies is solved, but the package will be huge

Linux
- easiest for developer, but not for user: let user build the package
- helpful tools:
-- cmake download_project can download and build the dependency (used in Mantid for googletest)
—- Conan: A package manager for C++. Packages are built using "recipe" scripts which are defined in Python and are cross-platform (Linux, Mac, Windows). Free public hosting of recipes is available and you can make use of many existing recipes created by other people. To avoid having to rebuild dependencies on developer machines it is possible to store binaries by using the free server software on your own server or paying for a cloud hosted service. Here is a short video from Jason Turner (of CppCast) on using Conan with CMake:
https://www.youtube.com/watch?v=9cCQHJ-cNHY
—- Ansible: A deployment tool which can be used to install/update software across the facility. Only requires that remote systems have a Python interpreter installed. Unlike other options, such as Chef and Puppet, it does not require running a server. Deployment scripts are defined in YAML.
—- Both, Conan and Ansible are being used for a range of projects at ISIS and the ESS.

- build rpm/deb package:
—- simplifies installation across the facility
—- not so easy to maintain (many different platforms, dependence on the packages which may be outdated in the system)

- all-in-one package (a self-contained application bundle that contains the application and everything the application needs to run), like for win/mac:
—- (-) no experience yet, the package may be large
—- (+) the package does not need installation, should work out of the box
—- helpful tools: appimage, linuxdeployqt
—- example of such package built by Juan: https://github.com/juanmcloaiza/AppImageExample

Packaging of documentation:
- pandoc — tool to convert between different documentation formats (latex, markdown, etcetera)

- the documentation should be kept under the version control
- the popular ways: hugo (BornAgain), readthedocs(MJOLNIR), .rst files packed as .html in the software package (Mantid, Sasview)

Optimization (Simon Ward)

This was a spontaneous discussion that turned out to be more popular than expected, with ~12 participants from all institutions.

- Firstly we explored what people currently use for optimization and found:
— SciPy optimizers were heavily used
— Optimizers from the Root library were also used

-We then discussed future optimizers:
— Bayesian statistics might be useful, but computation time is a problem as well as dealing with priors.
— Inspiration from the Cosmology community might be useful to investigate

-There was also a brief discussion on choosing the correct optimizer for the job and anticipation for the talk of Anthony Lim

-We also briefly discussed the gradient optimisers of Tensorflow and looked forward to the talk of Jonathan Fisher

Materials libraries (Gennady Pospelov)

Final WP10 deliverables (Thomas Holm Rod)