Report on Workshop I on coordination in SINE2020 WP 10 on Data Treatment

Group picture with the participants at Workshop I in WP10.

Venue:

Paul Scherrer Institut, Switzerland

Date

April 4 12:30 to April 5 15:00

Purpose

Coordination of activities

Participants

There were 27 registered participants of which 26 showed up. All partners and observers were represented at the meeting with the exception of the observers TUD and TUM.

Action point:

Facility specific requirements passed on to relevant technique responsible.

Deadline August 1, 2016

Executive summary

A workshop corresponding to Workshop I in the WP10 description was held at the Paul Scherrer Institut in Switzerland from April 4-5. Anders Kaestner from PSI and the WP10 Leader Thomas H. Rod from ESS organized the workshop. 26 persons participated in the workshop representing all participating facilities and observers in the work package except for the observers TUD and TUM. A mix of scientists, developers, and managers resulted in fruitful discussions and knowledge sharing between the development teams from the different participants, as well as between scientists and developers.

Brief status updates were given by represented observers and facilities followed with presentations on the programs that the work package focuses on (i.e. Mantid for data reduction, SasView for analysis of SANS data, BornAgain for analysis of reflectometry data, nMoldyn/MDANSE for converting MD simulations to scattering cross sections, and MuhRec/KipTool for analysis of imaging data) as well as current work on providing DFT based analysis software for muons and Task 10.2 on Standard and Guidelines. The workshop concluded with discussions and coordination for neutron scattering and neutron transmission techniques that took place in parallel. The conclusions from the presentations are that all the participants with sufficient funds to recruit staff specifically for this WP had recruited them by the time that the workshop occurred, i.e. ILL, PSI, FZJ, ESS, and ISIS and that at ESS, ISIS, and ILL, these staff will work in conjunction with other related projects and ongoing activities; Mantid project at ISIS, Endurance project at ILL, and the ESS project itself at ESS.

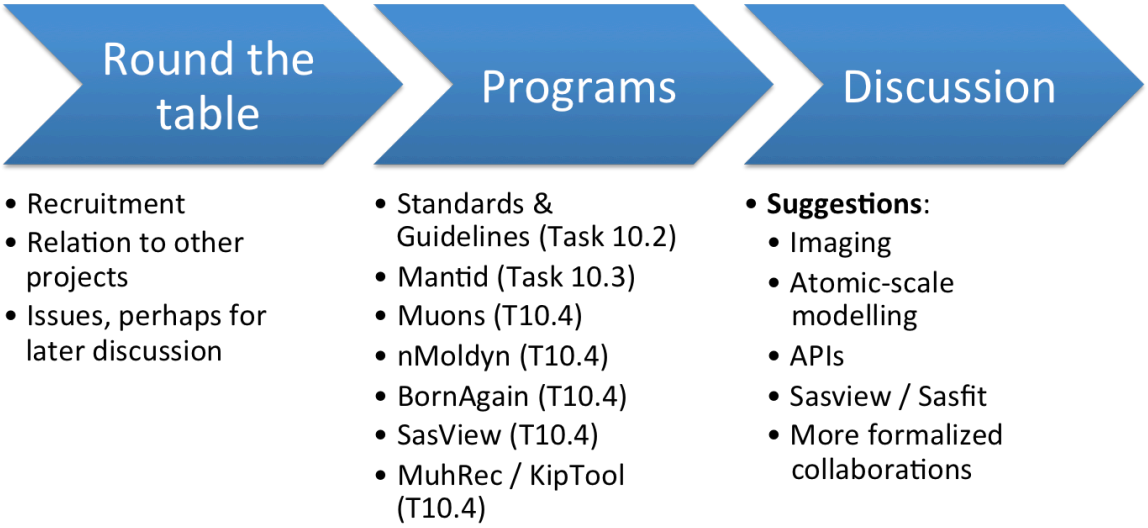
The techniques employed for the presented programs were strikingly similar pointing to an emerging software development standard within the field and hence favoring inter-operability. Programming languages are C++ and Python and graphical user interfaces are based on Qt or, in the case of MDANSE and SasView, wxpython. However, SasView is in the process of converting to Qt. Git is used as revision control system, GitHub as the repository host, and Jenkins for Continuous Integration, with the exception of BornAgain, which is hosted internally at MLZ and where TeamCity is used for Continuous Integration. MuhRec and KipTool are in the process of being converted to an open source project hosted on GitHub and with build servers hosted at ESS. Thus, there is preference for Python/C++/Qt open source projects hosted on GitHub and with Jenkins employed for continuous integration. With regard to creating DFT based analysis software for muons, it is worth noting that it is envisioned that that will be based on Mantid and the Atomic Simulation Environment (ASE), where the
latter also is an open source Python/C++ project. A summary of techniques employed for the different programs are provided in Appendix I.

At the end of the workshop there was a discussion among participants focusing on scattering in parallel with a discussion among participants focusing on imaging. The discussions led to an agreement that each facility gather requirements for each of the techniques considered in the WP and pass them on to the main responsible for that technique on August 1 at the latest, so that a presentation and discussion can take place during the SINE2020 General Assembly in September. The imaging people discussed the formation of an international advisory committee for imaging and will continue the discussion at a conference in Beijing, which unfortunately occurs during the General Assembly meeting.

High-level program

To foster the coordination and collaboration among the facilities a program for the meeting was developed consisting of three major parts:

1. Brief partner updates (5 minutes each, max 2 slides)
2. Presentations of each of the software programs that the work package will focus on
3. Discussions



Summary of Partner presentations (Round-the-table):

The partner presentations are summarized below:

1. Thomas Holm Rod, ESS

Has recruited Piotr Rozyczko with start January 1st and Wojciech Potrzebowski on February 1st and both contracts ending December 2017. They both work on Sasview, so ESS Sasview tasks will be completed before planned. Plan to hire a third person for six months with start September 2016 to work on imaging with Markus Strobl at ESS, Søren Schmidt at DTU, and Katia Pappas at TUD.

A related project is the Data Analysis and Modelling Work Package in the ESS construction project, which is based mainly on in kind contributions. ESS is working on getting reflectometry software provided by MLZ (as well as QENS and engineering diffraction) and Imaging software from PSI, thus leveraging SINE2020. Moreover, ESS Bilbao for diffraction and a yet to be determined partner for INS. The ESS Data Analysis and Modelling group also provides support for McStas primarily via Peter K. Willendrup, a DTU staff member who works part-time for ESS.

ESS has developed a good collaboration with the Sasview developer community and hosts their build servers.

The following members of the ESS Data Analysis and Modelling group participated in the workshop (primary work tasks in parenthesis):

- Piotr Rozyczko (Sasview, SINE2020)
- Wojciech Potrzebowski (Sasview, SINE2020)
- Céline Durniak (diffraction + QENS + reflectometry software)
- Torben R. Nielsen (SANS + INS software)
- Thomas Holm Rod (Group Leader)

Also from ESS:

- Jonathan Taylor (Group Leader for Instrument Data incl. Mantid work)
- Markus Strobl (imaging and engineering coordinator, ODIN instrument scientist) See 11 below.

2. Joachim Wuttke, MLZ/FZJ

Has recruited Jan Burle on SINE2020 funding with start November 2015, however various team members of the MLZ scientific computing group will work on the topic on extending BornAgain to also cover reflectometry besides GISAS. The scientific computing group supports all instruments at MLZ (regardless of affiliation) with data processing software. Current projects are BornAgain, software for Stress-spec, and Mantid for ToF instruments.

The following members of the scientific computing group participated in the workshop;

- Jan Burle (BornAgain, SINE2020)
- Jonathan Fisher
- Marina Ganeva (Mantid)
- Walter van Herck
- Gennady Pospelov (BornAgain)
- Joachim Wuttke (Group leader)

3. Anders Markvardsen, STFC/ISIS

ISIS is planning to have a flat spend profile and use a combination of existing resources from the Mantid development team as well as new recruits Karl Palmen who started January 2016 and works on Task 10.2 Standard & Guidelines together with Anders, and Thomas Perkins who will start ~December 2016 and will work on Muon related software as part of Task 10.4. Moreover, Federico Montesino Pouzols is responsible for Mantid imaging software.

Participants from ISIS were:

- Federico Montesino Pouzols (Imaging)
- Anders Markvardsen (Mantid)
- Stephen Cottrell (Muons)

4. Stephen Cottrell, STFC/ISIS and Pietro Bonfa, UNIPR

A brief status of Task 10.4 for Atomistic Modelling for Muon Spectroscopy was given jointly by Stephen Cottrell and Pietro Bonfa.

UNIPR recruited a PhD student Ifeanyi John Onuorah from November 2015 who will work on using DFT for modelling of muon spectroscopy under supervision of Prof. Roberto De Renzi as the UNIPR contribution to SINE2020 WP 10. Their work will be further complemented by work by post doc Pietro Bonfa who started January 2016 and is funded by UNIPR. They are planning to use Mantid as platform for hosting a Python library for site refinement and visualization tools and also on bringing muon groups working on DFT/dipole methods together via a workshop late 2016.

Pietro Bonfa was the only person participating from UNIPR. Besides Stephen Cottrell from ISIS participated.

5. Mark Johnson, ILL

Has recruited three programmers with funding from the ILL internally funded BASTILLE project and SINE2020. Moreover, they will have received one year of consultancy from Ian Bush at Tesella. The main focus in the beginning will be on Mantid development for ILL instruments including the ILL contribution to Task 10.3, which primarily will be on Mantid for SANS, powder diffraction and QENS (whereas PSI will be in charge of Mantid for reflectometry). Later in the project they will also spend a year of effort for handling of lattice dynamics simulations in nMoldyn/mdanse and a year of effort for QENS.

Mark Johnson was the only participant from ILL.

6. Emmanouela Rantsiou, PSI

Emmanouela Rantsiou is from the Neutron Optics and Scientific Computing group at PSI and and will work half-time with Mark Könnecke on Task 10.3 for four years. They will make Mantid the standard data reduction software at SINQ and will start with AMOR. Level of effort for SANS in Task 10.4 was currently unclear.

Emmanouela was the only PSI person participating from the scattering side of the project at PSI (see 8 below for other participants from PSI). Besides Joachim Kohlbrecher participated as an important SANS (Sasfit) stakeholder.

7. Frédéric Ott, CEA/LLB

LLB has two cold neutron radiography stations and their task in WP10 is to implement and test new computed tomography algorithms optimized for GPU and made available as plug-ins for MuhRec. The overall goal is to reduce the acquisition time.

8. Anders Kaestner, PSI

Has recruited Chiara Carminati from April 2016 to work on the imaging aspects of Task 10.4 for two years with Anders Kaestner. They will base their work on Muhrec, KIPTool, ImagingTool, and nGI tool.

Participants from the PSI imaging side of the projects were:

- Chiara Carminati
- Anders Kaestner
- Manual Morgano (see 11 below)

Moreover, Emmanouela Rantsiou also participated (see 6. Above).

9. Nikolay Kardjilov, HZB (observer)

Nikolay is an imaging instrument scientist at HZB, but also works with Bessy instruments. They have a number of homebrewed software solutions mostly developed in IDL, but some also in C++ that for instance address dark field imaging and polarized neutrons.

10. Søren Schmidt, DTU (observer)

Søren is a stakeholder/advisor for the ESS contribution to imaging and has a long track record in R&D for imaging analysis including combining diffraction data with imaging data to get detailed information about grains in crystalline structures. He also has an interest in including different modalities for analysis. Søren is a co-developer of FABEL.

11. Manual Morgani, PSI

Manual presented on behalf of Markus Strobl from ESS, who could not make it in time for this presentation.

An overview of ESS interests and requirements in the context of those of a broader European community was given. The need for an international advisory board for the imaging part of SINE2020 was stressed. The plan for the ESS/DTU/TUD 6 month's contribution (see 1) is to prepare the ground for ToF imaging.

Software Program presentations

Muons by Pietro Bonfa, UNIPR, and Stephen Cottrell, ISIS/STFC

Muon spectroscopy is complementary to neutron scattering and the two techniques are often used in a combined fashion.

The goal of the muon task is to investigate DFT based methods for the analysis of muon spectroscopy data and to make such methods available to the users in an easy and interoperable way. The idea is to use Mantid as a framework / host for fitting of simulated spectra that in turn are based on input from DFT calculations. It was furthermore discussed to use the Atomic Simulation Environment (ASE) as interface to various DFT codes.

Due to the overlap of the neutron scattering and muon spectroscopy community it is a clear advantage if the same data treatment tools (in this case Mantid) are provided for both communities. Moreover, it was pointed out that the needs of the muon spectroscopy community becomes increasingly similar to those of the powder diffraction community which was illustrated with the program BasIreps which is part of the Fullprof suite of programs. DFT is not currently sufficiently accurate and it was therefore suggested to use Bayesian statistics to evaluate different muon sites.

Moreover, as indicated in some of the neutron scattering talks, the usefulness of Bayesian analysis for dealing with uncertainties was emphasized.

In order to facilitate the development of useful DFT based methodologies a workshop is planned towards the end of the year that will gather all groups that develop DFT based analysis methods for muon spectroscopy. Moreover, they collaborate with the Theoretical and Computational Physics group within STFC Computing department on a two-year post doc position focusing on collaborative research projects with the muon spectroscopy community.

Guidelines and standards plus Mantid by Anders Markvardsen, STFC/ISIS

In this presentation the initial work on developing Guidelines and standards to be used by the rest of the project was discussed (Task 10.2), as well as the Mantid program for data reduction (Task 10.3).

Aspects of guidelines and standards have been addressed previously in NMI3-II and PaN-data. More specifically;

1. NMI3-II Data Analysis Standards (WP6) Task 2: solutions for developing a common software infrastructure (2014).
2. PaN-data (D2.2) Common policy framework on analysis software (2011).

The idea of standards & guidelines is to facilitate interoperability. At least two levels of interoperability can be envisioned;

- Low-level interoperability in the form of Plug-and-play. Different software components can easily be linked (e.g. Mantid fitting functions can be used in sasview).
- High-level interoperability where different programs can be easily linked. Examples are Mantid/McStas, GASA/Mantid, and Atomic Simulation Environment (ASE) that interfaces several atomic-simulation programs (e.g. VASP and CASTEP) and which also can be linked to Mantid or an analysis program.

In a broader term interoperability is in the context of SINE2020 simply the idea that software developed for one facility in the project can also be used by the other facilities in the project.

Focus of the low-level interoperability will be on fitting functions including Bayesian fitting and minimizers. Examples were given on pluggable fitting functions in Mantid. One example was the Bayesian fitting module Fitting Algorithm for Bayesian Analysis of DAta (FABADA). In the associated discussion it was mentioned that SASView also has a Bayesian fitting module in the form of BUMPS and that it should be possible to easily interchange FABADA and BUMPS as a practical example of (low-level) interoperability. A demonstration of how different minimizers can be tested and compared in a standardized and easy way is expected June 2016.

In relation to standards for data format is was mentioned that Nexus currently is the standard, but it is a standard that does not tell the users what they can expect to find in the file. It was therefore proposed that a standard for documenting data loaders should be introduced and implemented in all programs. Currently this is being done in Mantid.

On software development environments, current Mantid practice was compared with recommendations in the NMI3-II report. They are remarkably similar but a trend in moving from facility based hosting to cloud based was noted, specifically that local installations of Trac or redmine was replaced with github.

The Mantid project uses Coverity for static code analysis, has 8500 automated unit tests, ~300 automated system tests, 675 automated tests on scripts that are part of the documentation. Github is used for hosting of repository and issue tracker, Jenkins for continuous build and testing, and Sphinx for generating documentation.

The deliverable associated with Task 10.2 on Standards and Guidelines is due in Month 18, i.e. March 2017.

Nmoldyn and mdanse by Mark Johnson, ILL

nMoldyn = Computation and decomposition of Neutron scattering spectra from MOLecular DYNamics simulations.

MDANSE = Molecular Dynamics to Analyze Neutron Scattering Experiments

Mark first gave a historical perspective of nMoldyn that started as a Fortran 77 program published in 1995 by Gerald Kneller and co-workers, whereas the later nMoldyn 2, published in 2002, was based on Python and included Konrad Hinsen's MMTK library. nMoldyn 3 was a joint CNRS / ILL development involving Eric Pellegrini from ILL and included major code upgrade, task-farming parallelization capabilities based on PyRO (Python Remote Objects), new GUI and overall better performance, portability and usability. In a subsequent project, nMoldyn 4 was upgraded version so for instance the front (GUI) and back end were completely separated. Moreover, MDANCE was developed as an interface to nMoldyn 4 and McStas that enables virtual experiments to be performed. MDANCE is setup as a web service and has automated GUI generation and menu update for new analyses.

MDANSE uses Jenkins for continuous integration and GitHub and it is based on Python (incl. matplotlib), wxPython, and VTK.

1 year of effort will be spent on MDANSE at ILL as part of SINE2020 to enable MDANSE to read vibration frequencies and displacement vectors from DFT programs for the analysis of lattice dynamics and calculation of neutron scattering spectra from triple axis and time-of-flight instruments.

References:

1. nMOLDYN: G.R. Kneller et al, Comp. Phys. Comm. **91** 191 (1995).
2. nMoldyn 2: T. Róg et al, J. Comp. Chem **24**, 657 (2003).
3. nMoldyn 3: Hinsen et al., J. Comp. Chem. **33**, 2043 (2012)

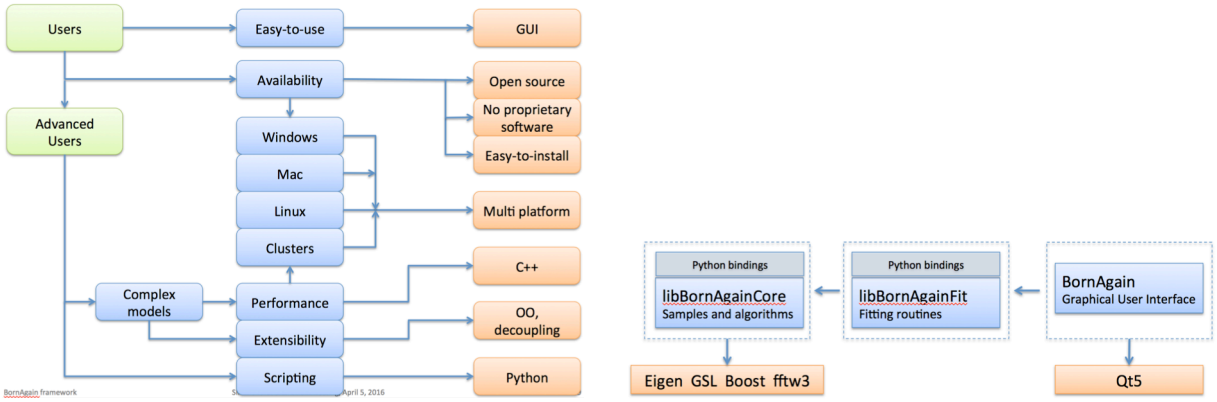


Figure 1. Left diagram shows the mapping of high-level user requirements that have led to particular technology and policy choices for BornAgain. The BornAgain high-level architectures is illustrated by the right diagram.

BornAgain by Gennady Pospelov, MLZ/FZJ

BornAgain is an analysis code developed for Grazing Incidence Small Angle Scattering (GISAS) that calculates intensities from known sample structures from the Distorted Wave Born Approximation. The code is solely developed by the MLZ Scientific Computing Group and supports the Maria and REFSANS instruments at MLZ that also need support for polarization and more sample geometries. Thus, BornAgain is envisioned to replace IsGISAXS which is not supported anymore.

Development started in April 2012 with Version 1.0 released in February 2015 and with ~200,000 lines of code (excluding SWIG generated ones?). As part of SINE2020 and the High Data Rate Processing and Analysis initiative, the Scientific Computing Group will extend BornAgain to also handle the more general specular reflectometry.

BornAgain is developed in C++/Python/Qt5 using SWIG for wrapping C/C++ to Python, is multiplatform (Windows, Mac, Linux, cluster), and open source (GPL3) and based on CMake. Doxygen is used for documentation, Coverity for static analysis, and googletest (330 tests) and QtTest (60 tests) for unit testing of the core library and GUI models, respectively. Repositories and build environments are hosted locally at MLZ.

It should be noted that the choice of SWIG was made after careful analysis of alternative solutions as well as testing of boost::python. SWIG supports both Python 2.7 and 3 and the generated code is portable (compiles with gcc, clang, and Visual Studio), adopts C++ doxygen comments as doc strings, among other things.

BornAgain is very well modularized (see Figure 1). From a user perspective, a user can work with BornAgain via a Python based scripting language or a GUI, which then in turn generates an executable script.

As mentioned the GUI is based on Qt5 and a Model-View-Controller (MVC) architecture as illustrated in Figure 2, on the right hand side effectively separating the user exposed part from what is being displayed. It was mentioned in the associated discussion that the Mantid development team had found it more suitable to move from an MVC architecture to a Model-View-Presenter (MVP) architecture.

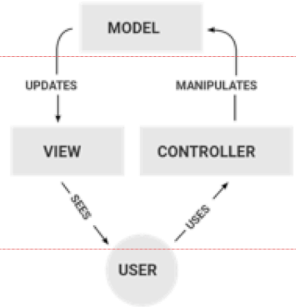


Figure 2. Model-view-controller (MVC) architecture employed for the BornAgain GUI.

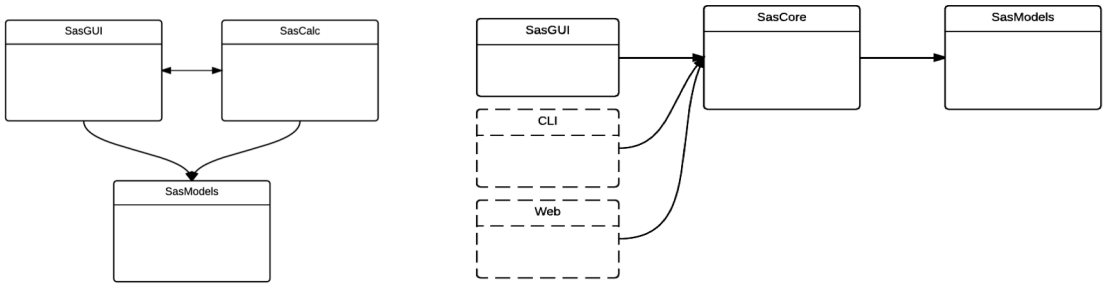


Figure 3 Untwinning SasView. Previous (left) and future (right) architecture for SasView with dependencies between the high-level modules. The SasCore module contains fitting algorithms that also can be run interactively via Python and SasModels contains sample models.

In BornAgain the following 3rd party code is used for the GUI;

- QCustomPlot (scientific graphics)
- Qt-manhattan-style (few styles/widgets borrowed from Qt creator code)
- Qt-propertybrowser-framework (dynamic property editors generation).

Besides the extension of BornAgain to also handle reflectometry, future work will involve the possibility to do fits in the GUI, representation of real samples using Qt3D, and adaption of Qt installer framework to create MacOS and Windows installers.

Sasview by Piotr Rozyczko, Wojciech Potrzebowski & Torben R. Nielsen, ESS

This presentation concerned two parts, namely 1) the ongoing work on Sasview (Piotr and Wojciech), and 2) live-analysis with Sasview (Torben).

SasView is used for analysis of small-angle scattering data and can handle both 1D and 2D data. It provides a number of sample models as well as different optimizers for the fitting including some based on Bayesian statistics. It allows for polydispersity and it is possible to add customized models. Besides 'traditional' model fitting it also supports inversion of the scattering pattern into real-space pair-correlation functions as well as the quantification of some model independent parameters; the scattering invariant, volume fraction, and specific surface area.

In a historical perspective, Sasview (originally called SANSView) comes out of the DANSE (Distributed Analysis for Neutron Scattering Experiments) in 2006 funded by the National Science Foundation in USA and with NIST and SNS as contributing facilities. From the end of the DANSE project most development took place during annual code camps until 2012 where a full time developer was employed at NIST. The code camps have continued until today where they now run twice per year. ILL and ISIS joined the collaboration in 2012 and ESS in 2014 and ESS recruited two developers in the beginning of 2016 as part of the ESS contribution to SINE2020.

Additionally, there are approximately 25 part-time contributors, mostly instrument scientists, and a management team consisting of representatives from NIST, SNS, ESS, and ISIS.

The management team has written a roadmap for SasView, which maps very well to the goals in SINE2020.

A focus area in SINE2020 is better modularization and modernizing of the GUI including converting from wxpython to Qt. To this end, the code is being refactored in order to remove dependencies between different modules and a new GUI is being developed that is based on pyQt thus

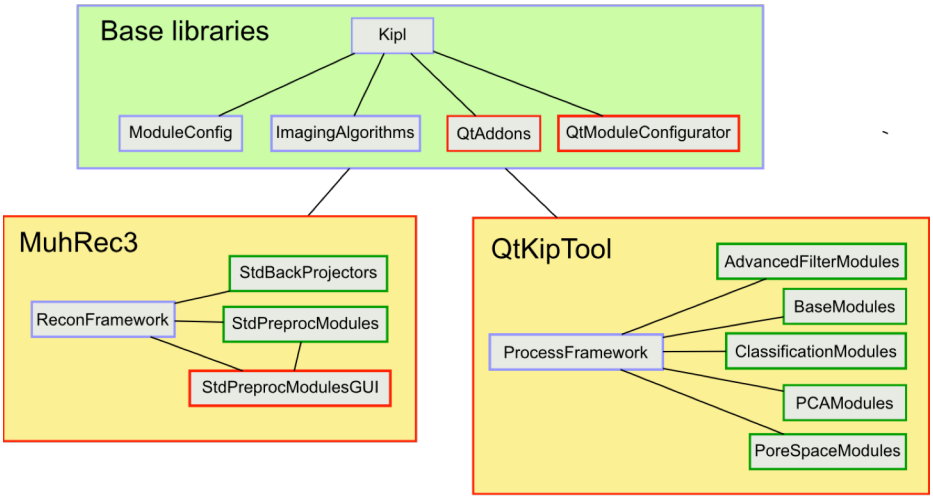


Figure 4. Architecture for MuhRec and KipTool.

facilitating interchanging components with Mantid and BornAgain. Moreover, it is the idea to extend the sasmodels library with models from sasfit.

With regard to live-analysis, a proof-of-concept for a Live-Neutron Data Analyzer (LiNDA) was demonstrated. The demonstrated prototype progressively fitted a sasview model (a sphere) to fake experimental data as they appeared using the fit package bumps also from SasView. LiNDA is well modularized and bumps can easily be replaced with other fit packages (e.g. lmfit).

Muhrec/KIPTool by Anders Kaestner, PSI

First an overview of the data processing workflow and existing tools used by the neutron imaging community was given. For imaging there exist excellent commercial software that are widely used such as Matlab and IDL for projection processing, Octopus for computed tomography reconstruction, and Matlab, VG Studio and Aviso for 3D processing, analysis and visualization.

For cases that are not covered by existing software, Anders Kaestner has developed MuhRec for image preprocessing and reconstruction and KIPTool for 3d image processing In addition it is intended to add ImagingTool for basic image combination and arrangement and at a later stage when the algorithms in nGITool are published this tool for neutron Grating Interferometry processing will be added to the tool palette. The tools are developed in C++ with GUIs based on Qt5 and with multi-threading primarily based on OpenMP. MuhRec and KipTool are built for Windows (64bit), Mac OS X, and Ubuntu 14.04. Unit test coverage and documentation are rather limited.

MuhRec and KipTool are rather well modularized and new modules can be added in a plug-and-play fashion at run-time, so that the image processing workflow can be fully customized. The next steps in SINE2020 are for MuhRec to add cone beam geometry and more features (e.g. iterative reconstruction methods and support for higher-dimensional data) and increase the general user experience (e.g. preprocessing time, stability, python scripting, improved user documentation). For KipTool the next steps are to add instrument related processing and more modules (e.g. for registration, segmentation, analysis, and quantification) and to add Python

scripting. Moreover, support for arbitrary number of dimensions as well a support for multi-dimensional data points will be added.

During the presentation it was emphasized that the best way to address higher-dimensional visualization is still an open question. There are some commercial, fully featured, but rather expensive tools available (e.g. VG Studio and Aviso) that still fail for some specific tasks (e.g. time series of volumes and vectors in 3D). These topics will be targeted during a workshop planned to take place in January 2017, which is funded out of COST action MP1207: *Visual analysis of dynamic processes* (i.e. funded by an internal PSI grant).

Discussions

Figure 5. Collaboration in action. People have gathered in small cross-facility groups in order to share knowledge and experiences and discuss common issues.

Neutron imaging

The discussions in the imaging group started with an overview how the participants treat their data at the different facilities. The first difference was already identified on the topic data formats and how experiment meta data are stored. This started a discussion about data format. All agreed that it is of interest to use common format(s) to store the data, it was however not yet agreed if we should continue using fits/tiff with either embedded meta data or start using the NeXuS format. The objective against NeXuS is the absence of tools (commercial and open source) that can be used efficiently with the format. The community is used to being able to look at single files and by clicking on them. Currently, only ISIS and the multipurpose test beamline BOA at PSI are using NeXuS as storage format. Still, it is a relevant format that should be supported. There will be a transition time were many formats will operate in parallel. Handling of meta data is related to the topic data storage. This is also handled differently at the different instruments represented at the meeting. In the future the aim would be to make use of this information in the processing and analysis and also to transfer the information with each step. To make this possible we have to agree upon a common way to store meta data.

The next discussed topic targeted the idea of common efforts to produce interoperable analysis software for neutron imaging. The current situation is that most facilities work with a mix of commercial and in-house developed software. There is currently no development collaboration and each group develops tools that perform essentially the same task, which is inefficient. The aim is to use a common open source repository to reduce work duplication and to provide a common interoperable suite of software for the processing and analysis of neutron imaging data. In order to make this happen it is of utmost importance that all involved partners provide

their input to the top-level requirements in written form. To formalize the structure for the information flow it was decided to organize an advisory group that meet on regular base.

Neutron scattering

The discussion was split into two parts: 1) Discussion of requirements gathering and inter-facility sharing of requirements to ensure inter-operability and 2) free discussions in smaller groups.

Requirements gathering

It was agreed that each facility should gather requirements from their own facility for each of the techniques considered in the work package and then pass them on to the partners responsible for the respective techniques. Thus, all partners should pass on requirements for analysis for SANS to ESS, for reflectometry to MLZ, for imaging to PSI (Anders), and for QENS to ILL.
Joachim K. suggested that the developers should visit the other facilities for longer periods (e.g. two weeks) in order to observe how they work at each facility but no final conclusion was made in this regard.

Actions points

Each partner captures requirements at their facility and pass on to relevant technique responsible. *Deadline August 1, 2016*

Appendix 1: Techniques employed for software development

	Mantid	BornAgain	SasView	MuhRec/KipTool	MDANSE	Muon SW
URL	mantidproject.org	bornagainproject.org	www.sasview.org (1)			
Lanugages	C++/Python	C++/Python	C++/Python	C++/Python	C++/Python	
Python<-C++		SWIG				
GUI	Qt	Qt5	wxpython -> Qt		wxpython	
Graphics	Paraview (2)	QCustomPlot			VTK(2)	
Repo	git	git	git	git	git	See Mantid (8)
Issue tracker	GitHub	Redmine	Trac (3)		GitHub	
Location of repo	GitHub	MLZ	GitHub	PSI -> GitHub	GitHub	
Loc. of build servers		MLZ	ESS	ESS (4)	ILL	
#Facilities	7	1	6	1	1	
CI	Jenkins	TeamCity	Jenkins	Jenkins		
Coding standards	Yes		Under development (5)			
Documentation	Sphinx	dOxygen	Sphinx			
Static analysis	Coverity	Coverity				
License	GPL3	GPL3	Open Source (6)	Open source (7)	LGPL3	
Windows			Windows 7			
Mac			OS X 10.9			
LiNUX			Ubuntu14.10			
Other platforms						

1 Note that there also is a sasview.org pointing to the SasView trac wiki

2 It should be noted that Paraview and VTK both are developed and sold by KitWare

3 The ESS contribution is managed with JIRA

4 Under planning

5 Where possible the Mantid guidelines are adopted

6 Different parts of SasView has different open source licenses

7 Is being moved to open source. The specific license is not determined yet.

8 The software is envisioned to be based on ASE, which interfaces to DFT codes, and Mantid, with development exclusively made in Mantid. ASE is solely based on Python.

Enclosures

Enclosure A: Programme

(Link to conference page: https://indico.psi.ch/conferenceDisplay.py?confId=4313)

Monday, 4 April 2016

12:30 - 13:30	Lunch & registration
13:30 - 13:40	Welcome
13:40 - 15:00	Partner presentations *Brief partner presentations on status and desired outcome of their participation in this work package. Observers are invited to inform about their interest.*
15:00 - 15:30	Coffee
15:30 - 16:15	Partner presentations *Brief partner presentations on status and their desired outcome of participation in this work package. Observers are invited to contribute.*
16:15 - 17:00	Muons *45'*
17:00 - 17:15	Break
17:15 - 18:15	Task 10.2 Standard and guidelines + Mantid *1h0'*
18:15 - 18:45	nMoldyn *30'*
18:45 - 19:00	Walk to OASE
19:00 - 21:00	Dinner (Restaurant)

Tuesday, 5 April 2016

09:00 - 09:45	BornAgain *45'*
09:45 - 10:30	SasView *45'*
10:30 - 11:00	Coffee
11:00 - 11:45	MuhRec/KipTool *45'*
11:45 - 12:45	Discussion & Coordination
12:45 - 13:30	Lunch
13:30 - 14:40	Discussion & Coordination
14:45 - 15:00	Closing remarks

Enclosure B: Participants

SINE2020 Workshop I in WP 10 on Data Treatment - Participant list

Venue & Date: Paul Scherrer Institute (PSI), April 4-5, 2016

Local organiser: Anders Kaestner (PSI)

WP Leader: Thomas Holm Rod (ESS)

List of Participants:

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Enclosure C: Organizational costs

Participants paid for their own travel and accommodation. Usage of meeting rooms were provided for free by PSI. Thus, the only cost to the workshop was for two times lunch, dinner, and coffee, that added up to CHF2260.90.