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WP5 Integrated User Access

Report on requirements for cross facility beam time access and strategy for implementation

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The complementary use of instruments using different probes (e.g. neutron, muons, x-rays, facility based AFM or electron microscopy) is extremely helpful in many scientific cases to obtain complete information about the investigated structures. Cross source access, the complementary use of instruments, laboratory services or infrastructures can support the efficient use of suites of instruments for users independent of the local institute. Therefore, platforms for cross facility beam time access might be useful for a lot of large scale facilities. At some NMI3 facilities individual solutions were established or are still under development.

The aim of this task is to give a survey of the existing activities at the NMI3 facilities and to discuss the experiences as well as new concepts to implement appropriate platforms within NMI3. The results will take into account comparable efforts by other communities (e.g. BioStructX, ESMI).

1. Survey of the existing activities at the NMI3 facilities

1.1. PSI

The Paul Scherrer Institute (PSI) operates three major user facilities for condensed matter research: a third generation synchrotron source (SLS), a medium flux spallation neutron source (SINQ) and the most powerful continuous muon source worldwide (SμS) with totally 2000 experiments and more than 5000 user visits each year.

In 2008 PSI launched a new initiative as service for users who are interested in a joint use of neutron and X---ray facilities for powder diffraction experiments. The initiative was meant to explicitly call for proposals that have a dedicated case for the joint use of both probes for a single scientific problem. As both probes are offered under one roof at PSI, the established procedure could serve as a kind of model system for cross facility beam time access.

Procedure at PSI

The call for proposals is launched once a year with a submission deadline, typically in February. The proposers may ask for beamtime on the thermal neutron powder diffractometer “HRPT” at SINQ and on the Materials Science beamline “MS powder” at SLS. Within the proposal the users particularly have to justify the need for both neutrons and photons for the specific problem. Afterwards, the proposals are evaluated by a referee panel that consists of members from both the “normal” SINQ and the SLS review panels. The evaluation of the combined photon and neutron proposals is processed entirely electronically (one database of the PSI Digital User Office “DUO”) without physical meeting of the review members, therefore the effort of the procedure is moderate.

Approximately 10% of the beamtime on both machines is being reserved for the combined photon and neutron proposals. Once accepted the proposals are scheduled in a row such

that the users only have to travel once to PSI for both experiments.

Statistics and experiences:
Since 2008 the call for combined photon and neutron proposals has been launched six times (no call was launched in 2011 because the MS powder beamline was being upgraded by then). Between 2008 and 2014 totally 71 proposals have been submitted, 37 (52%) could be accepted.

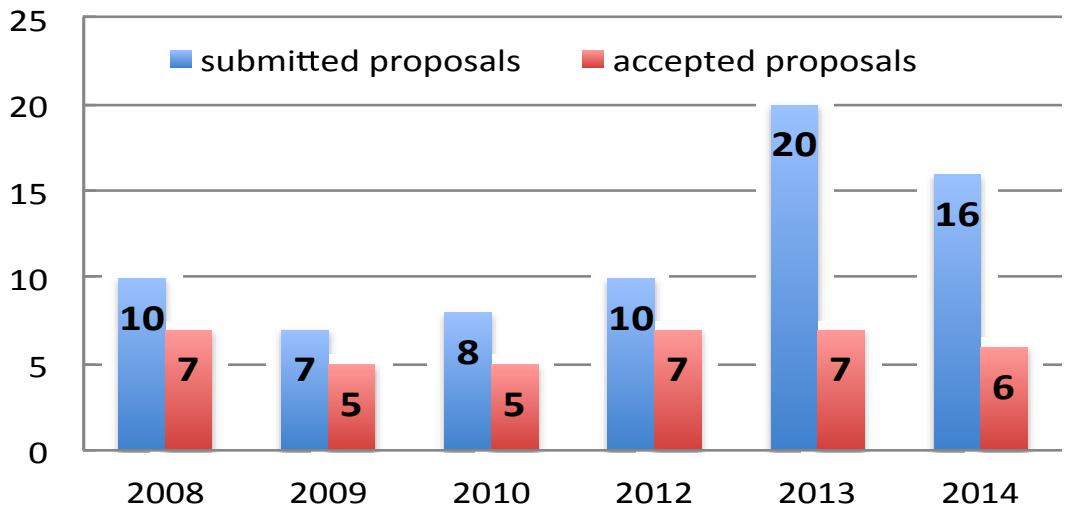

Fig. 1: Number of submitted and accepted combined photon and neutron proposals since 2008.

As can be seen from the chart above the call targets at a rather small community (10---20 proposals per year compared to typically 60-65 for MS-powder and another 60 for HRPT). Nevertheless there seems to be a clear request and a stable community. In 2013 the number of proposals has even doubled compared to previous years, which might indicate that a certain time is needed for new procedures to become popular, known and accepted in the community. The amount of allocated beamtime on the other hand could not be increased, which caused a larger overbooking in 2013 and 2014.

The chart below shows the number of allocated days and shifts (8h) over the last years, which is stable between 15-20 days and 20-30 shifts, respectively.

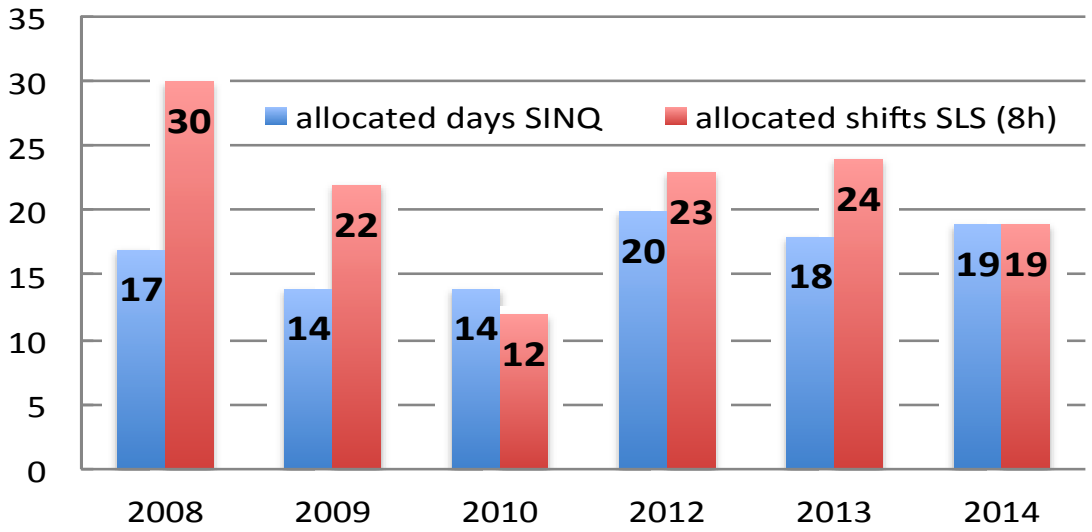

Fig. 2: Number of allocated days (SINQ) and shifts (8h, SLS) since 2008.

No serious obstacle could be identified so far during the whole procedure between call and experiment but it should be mentioned that this is also the result of a fair and open cooperation between the neutron and the photon powder diffraction groups at PSI.

Based on the very positive experience gained over the last years it is planned to continue the initiative. Other cross-facility combinations might be possible at PSI (e.g. imaging: TOMCAT and ICON, small angle scattering: cSAXS and SANS) but have not been further discussed yet.

2.1. ILL and ESRF

In the past the user offices of the Institut Laue-Langevin (ILL) and the European Synchrotron Radiation Facility (ESRF) tried hard to implement a system allowing the submission of joint proposals. Several scenarios with different complexity were identified and discussed. A general procedure for all instruments was not implemented, because too many technical implementations were necessary and a lot of practical questions had to be solved, e.g. the organisation of the safety procedure. Only a procedure for proposals for small-angle X-ray and neutron scattering (SAXS + SANS) experiments in the field of biology was established, running till 2010. As the number of proposals is limited, the effort for an IT-solution connecting both facilities is too high and the procedure is organised “by hand”. Nevertheless, a small but constant demand of the user community (20-25 proposals per year) was established during the last years in this field.

3.1. LLB

Propositions of offering the possibility of joined proposals between LLB and the synchrotron facility Soleil have been made several times, but were never achieved for two main reasons:

- Organisation is difficult due to different committees, deadlines, institutions and IT systems at the two facilities
- The number of interested users/projects is expected to be small.

About 8% of the total amount of proposals at LLB require more than one instrument. In the beginning, the user had to send only one proposal to request more than one instrument, but since more than 10 years the users have to send one proposal per required instrument due to organisational and statistical reasons (counting uncertainties, danger that proposal committee forgets to evaluate the second or third instrument mentioned in the proposal). For the second proposal it is enough to use the same text for the description of the science case so that copy and paste is possible. In every proposal the other proposals and corresponding requested instruments have to be mentioned. The current system is running fine and simplifies the administration of beamtime requests. Very seldom (around 1 case of 100) the link between 2 common proposals is getting lost (especially in cases when 3 instruments were requested).

4.1. GEMS

The German Engineering Materials Science Centre (GEMS) is the central user access platform to all photon and neutron instrumentation of the Helmholtz-Zentrum Geesthacht (HZG). GEMS instruments using synchrotron radiation are operated at PETRA II at DESY in Hamburg, instruments using neutrons are located at the FRM-II/MLZ in Garching. A main feature of GEMS is to fully exploit the complementarity of photons and neutrons in materials research. This includes the capability to provide users with combined neutron and photon beamtimes.

GEMS makes use of the existing state-of-the-art proposal application websites at DESY and MLZ which are fully integrated with the local on-site visit procedures and safety systems instead of coming up with a new GEMS proposal submission system for the GEMS instruments. In return GEMS is organizing the materials science proposal review panels both at DESY and MLZ and thus is fully integrated into the respective proposal review systems in its area of expertise. This is also the basis for offering GEMS-coordinated photon and neutron proposals at DESY and MLZ, allowing users to submit a proposal on one research topic in materials science to both facilities in parallel in cases where the complementary use of both probes is advantageous. This structure was developed only recently and presently there are long shutdown periods of FRM II and PETRA III. Therefore first experience with the procedure and acceptance of the user community will be obtained with the next call for proposals for beamtime at PETRA III in summer 2015 (deadline 1.9.2014).

5.1. HZB

HZB operates two large scale scientific facilities for investigating the structure and function of matter: the research reactor BER II, for experiments with neutrons, and the electron storage ring BESSY II, producing an ultra-bright photon beam ranging from Terahertz to hard X-rays. As both probes can be offered by HZB, a procedure for combined neutron and photon proposals was established with the aim to further strengthen the complementary use of neutrons and photons to help users to gain a more complete picture of matter.

At HZB the correlation of proposals for neutron and photon experiments is possible since 2009, since September 2013 the new GATE software allows the application for both probes in one single proposal without limitation in the number of instruments. For this purpose a joint submission deadline was introduced. One single review panel is rating the combined photon and neutron proposals. Between 2009 and 2013 a total of 111 combined proposals were

submitted. HZB monitors the option to consider if cross source independent beam time access is an advantage or not.

2. Discussion of concepts and new approaches

Cross facility beam time access can be an added value for the users and may enhance efficiency and output of user experiments, but needs a high administrative effort, because proposal systems of different facilities have to be connected and synchronised. Therefore, individual solutions were or are developed at the NMI3 centres or elsewhere.

The EU funded TNA Project **BioStructX** has offered a generalized access for the structural biology community to European synchrotron facilities and certain biology labs. The project established a single proposal submission entry point with a review panel supervising the scientific merit of the proposal. Most of the access was given on basis of the so called BAG proposal, allowing a group of researcher access to various facilities. The individual research group has to ask for individual access then at the facilities and the total amount of granted beamtime had to be monitored back by the project. The project has been adopted by many users in the field with several proposal rounds within the project lifetime till now. The drawback of the project is the individual beamtime allocation at the individual facilities which has not been coordinated and mismatch of access periods between project proposal deadlines and facility deadlines.

The European Soft Matter Infrastructure (**ESMI**) is an infrastructure project granted by the EU under FP7. ESMI offers all the relevant, world-class instrumentation for soft matter investigations. ESMI has established its own review panel, which assesses the scientific merit of all submitted proposals centrally within 4 weeks from the submission date. Two large-scale facilities (LSF) are ESMI partners, namely PSI, offering the SAXS instrument at the Swiss Light Source and FZJ, offering JCNS neutron scattering instruments at the MLZ in Garching, Germany. The overall request of ESMI instrumentation is rather high and in particular 38 proposals have been submitted to LSF, out of which 23 have been accepted. As ESMI is a new project some effort has been put in establishing the European soft matter community. After three years the awareness of the ESMI project is rather large being in total 216 proposals submitted. Despite of low amount of beamtime allocated by the ESMI review panel, this is very useful to the users, mainly due to the short waiting time between the proposal submission and performing the experiment.

With the EU funded **Science Link** project a new approach to involve industry in the use of large scale facilities has been taken. Industrial customers could apply for commercial beamtime via Science Link which funds the industrial use of the participating research infrastructures (PETRA III, GEMS, BESSY II, BER II and Max-Lab). Science Link is a good example for cross facility beam time access. In this project a central review committee decided which probe was the best for the proposed study and directed the proposals to the best suited instrument at one of the facilities. With more than 60 submitted and 47 accepted proposals in 3 calls (70 % SMEs) the Science Link project was very successful.

The facilities within NMI3 try to keep the necessary effort as small as possible. Separate calls for cross facility proposals for a small amount of beamtime at the instruments, the application for several instruments and additional services or infrastructures in one proposal and the

implementation of a review process with electronic workflow are used and proposed here. A successful approach is to limit the procedure to certain methods and user communities, like the combination of SAXS and SANS in the field of biology.

Possible procedures have to fit to the business model of the centres and have to be acceptable in terms of effort, administrative and safety issues. The facilities need a control tool and feedback system about the used beamtime. New strategies like by block allocation (BAG) of experiments or mail-in sample programs across sources have to be adopted and developed to enhance the flexibility of the existing systems. Thematic oriented calls in view of the Horizon 2020 strategy can also be considered for a successful strategy. Additional benefit for the facilities, like a growing user community and increasing quality and number of publications, will help to pave ways for cross facility beam time access, so that the centres get interested and agree to invest necessary resources to operate in these new concepts.