nmi3

Deliverable Number: D 5.8

Deliverable Title: Feasibility study on software prototype for cross facility beam time access

Delivery date: 31. 01. 2016 [month 48]

Leading beneficiary: HZB

Dissemination level: Report

Status: done

Authors: Thomas Gutberlet, FZJ

        Nils Leidel, HZB

Project number: 283883

Project acronym: NMI3-II

Project title: Integrated Infrastructure Initiative for Neutron Scattering and Muon Spectroscopy

Starting date: 1st of February 2012

Duration: 48 months

Call identifier: FP7-Infrastructures-2010

Funding scheme: Combination of CP & CSA – Integrating Activities

WP5 Integrated User Access

Report on feasibility study on software prototype for cross facility beam time access

T. Gutberlet, Forschungszentrum Jülich
N. Leidel, Helmholtz Zentrum Berlin, Germany

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. In the "Report on requirements for cross facility beam time access and strategy for implementation" (Task 5.5, Deliverable 5.7) administrative procedures currently existing at single facilities (PSI, HZB, ILL, ESRF, LLB, GEMS) and European I3 projects with cross facility access (BioStructX, ESMI, Science Link) were presented. The report emphasized that it will be important to keep any administrative efforts as small as possible for establishing possibilities for cross-facility access.

Possible procedures have to fit into the business model of the centres involved and have to be acceptable in terms of effort, administrative and safety issues. The facilities need a control tool and a 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.

Based on these boundary conditions a software prototype was developed to demonstrate the administrative and practical feasibility to offer and manage cross-facility beam-time access. The functionalities required in this software prototype are added to the software prototype developed for harmonized proposal form submission and review between facilities (Task 5.3, Deliverable 5.4) and are described in the following.

This software prototype covers, as a feasibility study, a web-based online proposal handling system, which allows the generation of facility-specific standardized proposal forms, the submission of proposals to selected facilities, future editing of downloaded proposal files, cross-beam time monitoring and peer review on a basic level. Each facility can determine what data is required and can add and remove fields to the proposal form. Cross-facility beam-time access is monitored by linking the cross-facility proposals via a specific marker. The facilities can manage their own beam time and can see the allocated and used measuring time from the other linked facilities. The facility administrator can select referees for proposal reviewing. The reviewer can read and rate the assigned applications. A detailed description of these functionalities is given in the report D5.4.

In the following the added functions to manage cross-facility beam-time access are described. A working demonstration of the prototype is accessible in the internet under the URL http://nmi3.eu/proposal/. The software prototype is written in PHP version 5.5.5-dev and HTML connected to a MySQL database community server (version 5.6.15-log). For pdf creation the mPDF v5.7.1 PHP class is used.

Proposer:

- Proposal submission

The proposer can select the facilities where he/she wants to hand in a proposal and press the 'Choose facilities' button after selection. Multiple selection for cross-facility access is possible. A harmonized proposal form is created with all necessary fields according to the chosen facilities. Also an attachment may be added. After completion of the harmonized proposal form it is possible to download the proposal form as XML file for later editing or to submit the proposal form to the selected facilities. It is possible to upload and submit a previously saved proposal XML file to the selected facilities. After a control page, whether all fields are correctly filled in, one can submit and upload the proposal form.

- Own proposals

A summary table of all submitted proposals with information like proposal ID, proposal title, used instrument, allocated measuring time and the cross-facility code is shown. The proposer has the option to download the submitted proposals as XML file for later editing or as pdf file. It is also possible to add publication records to selected proposals.

Facility manager:

A facility manager sees the navigation menu below, where he is free to administer and manage proposals for his facility and monitor cross facility proposals and beam time access:

- SPF (Standarized proposal form)

The administrator may select, which information is necessary (Y = required, N = not required) to fill out in the proposal form, which is displayed to the proposer who wants to make an application to the facility. It is also possible to add additional fields to the proposal form to fulfill the special needs of each individual facility.

- Instruments

One can add further instruments to the facility list of instruments. This instrument list is available to the proposer. The proposer can select one or more instruments and can add them to the proposal. The facility manager can also select a person from the list of registered users in the database to appoint them as instrument scientist. This is necessary for the local technical reviewing, therefore corresponding instrument scientists have to be registered in the user database.

- Panel

The facility manager can add and edit the selection panels. And also can assign a person from the list of registered users in the database as members of the different selection panels.

- Facility proposals

For each proposal, one selection panel and one or more referees may be assigned. Each assigned referee is able to read and rate the proposal.

The table 'Ranking and measuring time' shows all proposals that have been submitted to the facility. It contains the proposal number, proposer name, title of the experiment, calculated averaged ranking and requested beamtime. It is also possible to allocate beam time hours to the proposal. It also shows the assigned reviewers and the score given.

To each proposal, a unique cross facility code is assigned. The code is necessary to monitor cross-facility beam-time access. The proposer has the ability with this code to mark cross-facility beam-time proposals additionally.

Add a panel:

Panel name [_____] [Add panel]

Edit panel data:
[P1 ▾] [Edit panel]

Facility: HZB

Please select the referee committee.

Name	Panel	
Ella Fitzgerald ▾	P1 ▾	[Select]

P1

Charlie Parker	[Delete]
Ella Fitzgerald	[Delete]

P2

Duke Ellington	[Delete]
Count Basie	[Delete]

Ranking and measuring time

Prop. ID	Proposer	Title	Ranking	Instrument	Req. beamtime	Alloc. beamtime	Cross fac. code	
3	Prof. Charlie Parker	Rapid X-ray photoreduction of dimetal-oxygen cofactors in ribonucleotide reductase.	Not yet rated.	HZB Inst 2	7	[_____] [Save beamtime]	5580240beefbc	[Edit cross fac. code]
Rating: Nils Leidel			0					
1	Nils Leidel	Bridging-hydride influence on the electronic structure of an [FeFe] hydrogenase active-site model complex revealed by XAES-DFT.	9.50	HZB Inst 1	5	5.00 [Save beamtime]	55801e6f316c1	[Edit cross fac. code]
Rating: Charlie Parker			9					
Rating: Duke Ellington			10					

- Proposal pool

The Proposal pool shows proposals, which have already been reviewed and are available for other facilities to take over. The author of the proposal can accept or reject the takeover by the new facility. After acceptation of the proposer a new technical review or a new general review may be done by the referee of the new facility.

Proposal pool

Proposal ID	Proposer	Title
4	Nils Leidel	Hydride binding to the active site of [FeFe]-hydrogenase.
		Added: 16.06.2015 - Origin: SINQ

Referee: Final grade: 9.00
Count Basie: 9.00

SINQ comment: [No comment available.]

Proposal status: TRANSFER POOL [Transfer proposal to HZB]

- Used beamtime

This table shows an overview of all proposals with important proposal data placed at the facility. Proposals with cross-facility beam-time access are linked together and have the same background color. The facility administrator can monitor the requested and allocated beam time from the connected proposals. Also an overview table of all summed allocated beam time per instrument and proposal round is shown.

Cross facility measuring time administration.
(Linked proposals have the same background color.)

Proposal ID	Facility	Proposer	Title	Instrument	Requested beamtime	Allocated beamtime
2-2015						
3	HZB	Prof. Charlie Parker	Rapid X-ray photoreduction of dimetal-oxygen cofactors in ribonucleotide reductase.	HZB Inst 2	7	
1	HZB	Nils Leidel	Bridging-hydride influence on the electronic structure of an [FeFe] hydrogenase active-site model complex revealed by XAES-DFT.	HZB Inst 1	5	5.00
2	SINQ	Nils Leidel	Bridging-hydride influence on the electronic structure of an [FeFe] hydrogenase active-site model complex revealed by XAES-DFT.	sinq instr	10	

Allocated beamtime hours per instrument

Instrument	Allocated beamtime hours
2-2015	
HZB Inst 1	5.00
HZB Inst 2	0.00
HZB Inst 3	0.00
HZB Inst 4	0.00

Referee:

	Logout	Referee Review	Messages
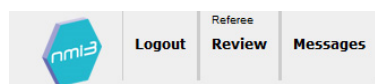
A list of all proposals to be evaluated by the reviewer is displayed. The reviewer has the option to assign a grade, give a comment or to reject a proposal. By hitting the button "Message to proposer" it is also possible to get into direct contact with the proposer via the internal messaging system. The message is anonymous to keep the confidentiality of the reviewer and copied to the attendance of the corresponding facility manager. The messages are stored in the system. In the "Show panel proposal" section all proposals from the selection panels, where the referee is part of, are shown. The instrument list shows every available instrument from each facility.

Please review the following proposals

Proposal	Proposer	Proposal title		Instrument Ranking
HZB 3 Feasible: No HZB comment: Instrument scientist: (HZB Inst 2) Recommend beamtime: 5.00 Comment: Message to proposer	**Prof. Charlie Parker** No comment available. good proposal	Rapid X-ray photoreduction of dimetal-oxygen cofactors in ribonucleotide reductase.	HZB Inst 2	Not yet rated. ▼ Submit A+ A A- B+ B B- C+ C C- D Not yet rated. Reject

Conclusions

This software prototype was developed as a comprehensive and at the same time most flexible tool for managing cross-facility beam-time access. It is designed to be as compatible as possible with the existing user administration systems of the large-scale facilities. This was ensured by involving the responsibles of the user offices of the neutron and muon facilities in Europe during the development of the program. Also the input of the user query performed at the beginning of this project was considered. The resulting prototype shows the feasibility but also the complexity of this approach.

Organisation of workflow of cross facility beam time access

- **Workflow facility and single user**
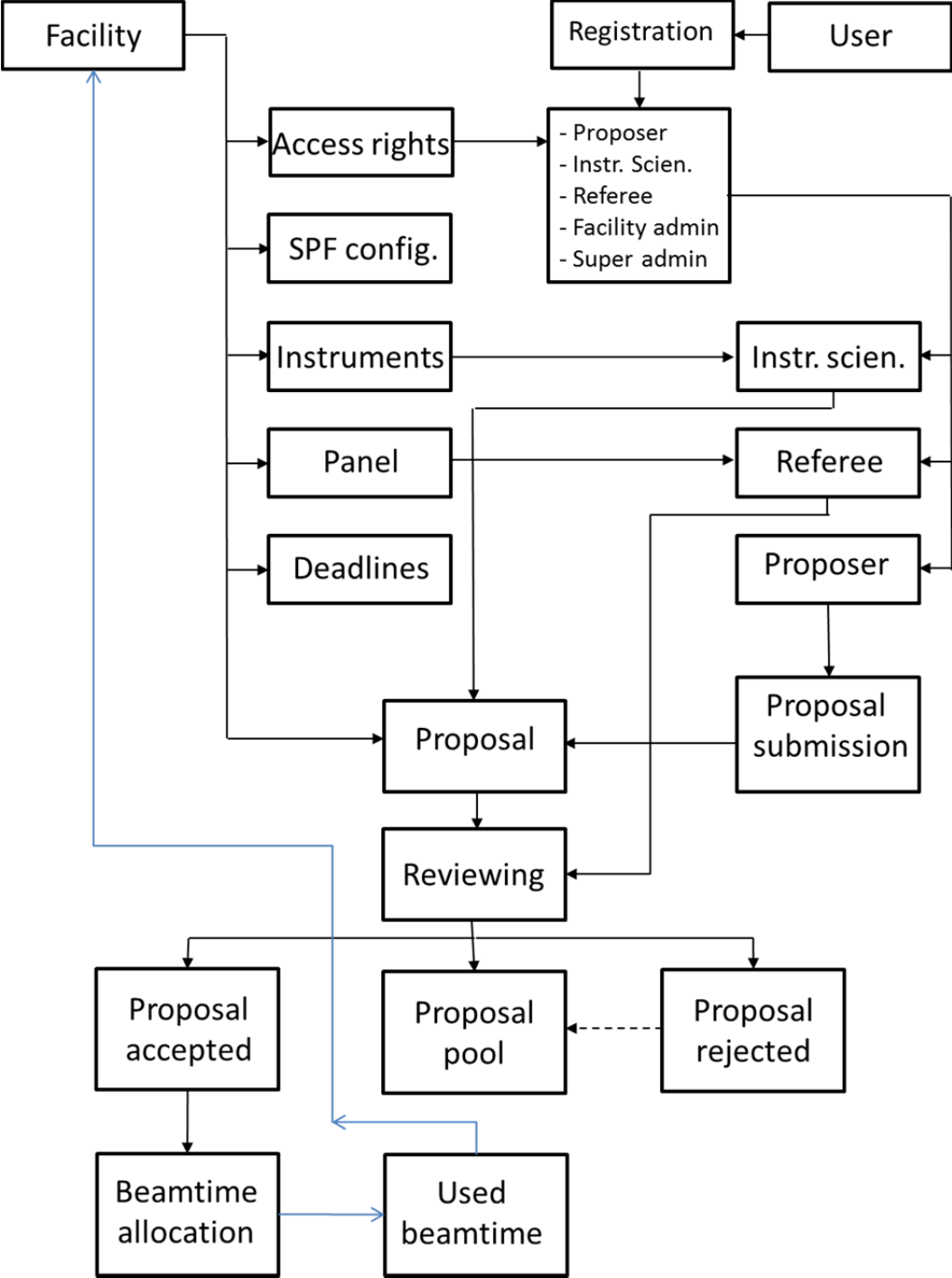
- **Workflow multiple facilities, reviewing and proposal and beamtime handling**