1. Introduction

The Work package 9 has now been completed. The goal was to study the feasibility of a generic, standard and flexible information system for managing the workflow from the scientific proposal to the publication in order to cope with the substantial increase expected in the number of users and their requirements in terms of experiment proposal management, sample tracing, metadata catalogue management and new possible rules of access. The feasibility study had to include discussions with most of the national synchrotron radiation (SR) laboratories to assess the feasibility of a European wide user data base of photon and neutron scientists and to analyse the potential for software development collaborations. It was agreed from the beginning that in the unlikely case that discussions with national SR laboratories show that there is no interest for a common software development; the ESRF would be the only case study.

The study had:

a/ To report on the existing software packages and their functionalities at the ESRF and national SR laboratories.
b/ To evaluate suitability for the ESRF
c/ To report on tools, technologies and methods used.
d/ To produce the specification of a generic, standard and flexible information system for the scientific user community. The document would have to describe in detail the implementation of such software at the ESRF (in eventual collaboration with other institutes).

The two workshops organized and the work carried out since the beginning of the study have provided the following reports:

Deliverable 9.1 : Software components and functions currently implemented at ESRF.
Deliverable 9.2 : Report on software components currently existing in partner institutes.

This last report aims at describing the specification of the future SMIS. It includes the partnership with other institutes in view of having a European SMIS system.
2. **Outcome of the partner institute visits**

Visits to partner institutes showed that most of them already have a software application similar to the ESRF SMIS. Report on visits is included in the deliverable 7.2 (Report on software components currently existing in partner institutes).

The table below gives a brief overview of features already implemented by the different systems.

<table>
<thead>
<tr>
<th>Laboratory name</th>
<th>Application name</th>
<th>Management of users</th>
<th>Management of laboratories</th>
<th>Management of proposals</th>
<th>Management of samples</th>
<th>Parameters for experiments</th>
<th>Scheduling of experiments</th>
<th>Experiment organization</th>
<th>Experiment safety</th>
<th>Experiment data</th>
<th>Experiment reports</th>
<th>Experiment statistics</th>
<th>Remote control</th>
<th>Access control</th>
<th>Computerized</th>
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**Legend:**
- Computerized
- Partially computerized
- Not computerized
The table below gives a brief overview of technologies used by the different systems.

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<thead>
<tr>
<th>Laboratory name</th>
<th>Application name</th>
<th>Cloning date</th>
<th>Oracle database</th>
<th>MySQL database</th>
<th>PHP</th>
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<th>J++</th>
<th>Java - Jsp - servlets</th>
<th>Java - Struts</th>
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<th>Workflows and Queues</th>
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(*) old version  
(**) new version

The two tables above clearly show that partner institutes already have their own systems. It also shows that technologies are different.

Visits showed an unpredictable overlap between the Work package 9 study and another study called EuroFEL also financed by the Seventh Framework programme. Several discussions and meetings have taken place and it has been decided to set up a specification on the minimum that can be done. The target is to specify a portal infrastructure proving a single user entry point for photon and neutron scientists. This portal infrastructure will be called Unified User Umbrella.
3. **Outcome of the workshops**

The first workshop held in October 2008 clearly showed that institutes were not ready to replace their existing systems by a new one in the short term. However, they expressed their concern to support and improve their application independently. They also agreed to begin cooperation in view of federating software developments. Three working groups have been set up:

- Publication tracking
- User & affiliation management
- Online proposal submission & beamline allocation

The goal of these working groups is to specify what would include a common application for these three subjects.

In order to help participants to communicate, a Wiki server has been set up (evuo.esrf.eu).

The second workshop held in June with partner institutes decided on a first approach for cooperating. The goal would be to set up a European Portal in view of having a European User database. It indicates clearly that in the short term, partner institutes continue to improve their own system.

4. **Overlap with the work package 7**

The work package 7, another project managed by the ESRF Computing Services, aims at providing “a single entry point for users coming on the ILL/ESRF site”. It consists in specifying and implementing a site portal mock-up. This site portal will group the common information of site facilities. It will also provide a common entry point to users for submitting proposals. This study will be described in detail in the deliverable 7.3 planned for November 2009. The overlap with the work package 9 is on the common entry point to users for submitting proposals.
5. **Specification of the future SMIS system**

Based on visits, workshops and the outcome of the work package 7, the specification is now split into three parts. The first one specifies the European Portal called “Unified User Umbrella”. The second part specifies the site portal including the connections to the ILL and ESRF SMIS systems. The third part specifies the improvement planned in the existing ESRF SMIS.

The initial aim of this study was to specify a generic system for all facilities. For reasons expressed previously, the generic characteristics for all institutes have been reduced to the Unified User Umbrella level. The generic characteristics of the site portal that will be described in the second part of the specification only concern institutes present on site (ILL, EMBL, ESRF). Finally, the third part of the specification concerns essentially ESRF. The picture below summarizes these three levels.
6. Specification part 1: The Unified User Umbrella

6.1 Introduction

Before describing the specification in detail, the objective of the overall project can be subdivided into three subsets as follows:

a. **Short term objective (within the next two years)**

Set up of a mechanism providing a unique ID to European facility Users. The ID delivery must be fast (a couple of minutes), self managed by users, without any approbation workflow, and reliable enough to avoid double entries for the same user.

Set up of a Unified User Umbrella (U³) grouping general information from facilities and offering links to local facility applications (proposal submission, report submission ...).

Set up of a European Single Sign-On (SSO) mechanism to access the central point (U³) and also local facilities. It must be based on the unique user ID mentioned at the beginning of this paragraph.

Remark: in the rest of the paragraph, Unified User Umbrella will be called U³.

b. **Medium term objective (within the next five years)**

Specification of a common look and feel for identical applications (proposal submission, report submission...).

Specification of common data formats (proposals, reports, samples ...).

Development of tools to import and export data. It will provide the possibility to submit the same information to different facilities several times.

c. **Long term objective (within the next ten years)**

Specification and development of non strategic and non competitive software applications (cross facilities proposal/report submission, event & workshop organization, ...).
6.2 Specification of the short term objective

6.3 Overall view

This specification is focused on the short term objective described previously. The general principle is that a user who needs to interact with a local facility goes through the U³ (Unified User Umbrella). Then, based on information stored in the U³ database, he is automatically redirected to the corresponding local facilities. The U³ is also a place where he records his non strategic personal data. Thanks to that, he can easily input this data to local facilities’ databases without having to enter the same information several times. Moreover, the U³ is a central point populated with public information coming from facilities (workshops, conferences, events, link to local user office applications ...). Finally, a Single Sign-On mechanism provides a comfortable way to access local facility applications. The following picture gives an overview of the user’s portal interactions.

![Figure 1](image)

6.4 Data protection requirement

As most facilities are financed by their country, the U³ must not provide information on the facilities’ activity. Sensitive information must be stored locally in facilities. Nevertheless, to provide a common attractive tool, the U³ must store information on users, affiliations and public information coming from facilities.
6.5 Common User ID database

For the time being, a user having an account in a local facility is identified by a local ID number. Consequently, he has a specific ID for each facility. A common ID is necessary for the U³. For obvious reasons we cannot remove local IDs. We therefore have to find a way to link the common ID with local IDs. Due to data protection requirements, the link between the local ID and the common ID will be stored in local facilities’ databases. That implies that each facility will add a complementary linking field to its local database. The figure below summarizes this mechanism.

![Diagram of Common User ID database]

**Figure 2**

Technical remarks:

- As we need to keep the list of facilities in which the user has an account, this information will be stored in the U³ (see e.g. User’s list of facilities).
- The local user management module must be adapted. This adaptation is described in chapter “Workflows”.

---

D. PORTE, ESRF – October 2009
6.6 **Common User Table description**

The Common User ID database can be easily managed by a relational table. The figure below specifies how this table could be implemented.

![Figure 3](image)

**Mandatory fields**

- **European_User_ID**: 1002
- **First name**: Dominique
- **Last name**: Porte
- **email**: porte@esrf.fr
- **AffiliationID**: 20
- **Birth date**: 06/05/1957
- **Login**: Porte.dominique@gmail.com

**Optional fields**

- **Gender**
- **Title**
- **Nationality**

Remark: It is important to define precisely how fields are generated and what is the character set. Concerning the first name and the last name, if we authorize a character set including French characters, due to the accents, the probability of mistyping is high and consequently multiple entries for the same user will be frequent.

6.7 **Common Affiliation ID database**

As for users’ ID, for the time being, each facility has its own affiliation database. The goal is to create and maintain a common affiliation database. It will be stored in the U^3. It will provide a common spelling for affiliations. As for users’ ID, for data protection requirements, the link between the local affiliation ID and the common affiliation ID will be stored locally in facilities’ databases. This implies that each facility will add another complementary linking field in its local database. The figure below summarizes this mechanism (green links).
Technical remark: The local user management module must be adapted. This adaptation is described in chapter “Workflows”.

Figure 4
6.8 Common Affiliation Table description

The Common Affiliation ID database can be easily managed by a relational table. The figure below specifies how this table could be implemented.

<table>
<thead>
<tr>
<th>European_Affiliation_ID</th>
<th>20</th>
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<tbody>
<tr>
<td>Acronym</td>
<td>ESRF</td>
</tr>
<tr>
<td>Name</td>
<td>European Synchrotron......</td>
</tr>
<tr>
<td>Address</td>
<td>2 rue Jules......</td>
</tr>
<tr>
<td>Country</td>
<td>France</td>
</tr>
</tbody>
</table>

Optional fields

<table>
<thead>
<tr>
<th>Official Web site URL</th>
<th><a href="http://www.esrf.eu">www.esrf.eu</a></th>
</tr>
</thead>
</table>

Figure 5

6.9 User’s list of facilities

In order to keep the list of facilities in which the user has an account, a list will be created to store this information in the U3. It could also be easily managed by a table with two fields, one for the Common user ID and the second for the ID of the facility in which the user has an account. Obviously, if the user is known in several facilities, he will have several records on this table.
6.10 Workflows

The following specifies how the portal and local facilities must behave in the different situations.

First scenario: The user accesses the $U^3$ for the first time. A screen proposes to create an account. He provides his first name, last name, date of birth, email, main affiliation. He has two possibilities to record the affiliation. Either it already exists in the common affiliation database, or he proposes a new one. In the second case, the new affiliation is recorded in a temporary database. It will be checked later on by a facility from the corresponding country.
Second scenario: The user already has an account in the $U^3$. He is connecting for the first time to the local facility B. There are two possibilities: Either he already has an account in the local facility B, or he is connecting to this local facility for the first time. In the first case, the local system must check that a link exists between the local user ID and the common user ID. Moreover, the local system must check if a link exists between the local affiliation ID and the common affiliation ID. Finally, the local facility is added in the $U^3$ “User’s list of facilities” for this user. In case a link does not exist, the local system must provide an easy way to create these links. The goal is to create links drawn in green and red on figure 4.

Significant remark: It is important to note that links between the local user ID or the local affiliation ID and the common user ID or the common affiliation ID are stored locally in facilities’ databases. This means that somebody reading data stored in the $U^3$ cannot know the local user IDs. It is only possible to see where the user is known.

6.11 Complementary $U^3$ features

In addition to the features described in the previous paragraph, the $U^3$ must provide the following features:

- Mechanism to check if a user already exists. When a portal gives the possibility to create one’s own account, multiple entries for the same user is a frequent problem. Sometimes, people prefer to create a new account rather than reusing an account they have already
created. This is mainly because they have forgotten their login or/and password. To be efficient, the mechanism checking multiple entries needs information. This is one of the reasons why several types of personal information is requested to create a new account (first name, last name, birth date, email, affiliation).

- Mechanism to retrieve a login or/and a password. This is a common feature provided by most portals. The user provides his email; he is emailed back his U³ login/password.

- Mechanism to merge accounts. When a user has mistakenly created several accounts, this feature provides the possibility to merge his different accounts. He gives the different logins/passwords to merge. One of them must be designated as the new official login/password.

- Mechanism to delete an account. To do so, the user provides his login and password.

- Mechanism to update personal data. The user must be able to update his first name, last name, date of birth, etc...

- Mechanism to input account modifications to facilities. Modifications like merge of accounts must be spread to local facilities.

6.12 Authentication and Single Sign-On

Most local facilities already have a portal. Moreover, most of them have already implemented a local AAA (Authentication, Authorization, and Accounting) mechanism. Merging all AAA mechanisms is unrealistic. Nevertheless, having a common authentication should be possible. Consequently, when a user logs in to the U³ and accesses a local facility, he does not have to login again to the local authentication mechanism. A Central Authentication Service (CAS) tool from YALE University could be a technical solution. However, so as to run all facilities smoothly, the same tool should be used.

In any case, local facilities should keep a local authentication mechanism for users without a U³ account, and authorization and accounting should remain managed locally.
6.13 **Technical implementation**

During the brainstorming held in Zürich on Wednesday, June 24 2009, several technologies were presented (Shibboleth, OpenID, Grid Certificate, CAS, CMS portal). The main goal was to evaluate which one could best match our U³ requirements. No final conclusion was taken. The subject still needs to be discussed.

6.14 **Roadmap**

This first milestone is the finalization and the approbation by facilities of the “Specification of the short term objective”. Then, an evaluation of the different technical possibilities should be organized. For example, we could set up several mock-ups in view of comparing the different solutions. This will require resources and a precise framework to manage the project. Again, a strong commitment from facilities will be mandatory. Finally, an official Unified User Umbrella could be launched. All that could be completed in less than two years.
7. Specification part 2: “a single entry point for users coming on ILL/ESRF site”

7.1 Introduction

As decided during the workshop held in May 29, 2008 at the ESRF, a working group composed of people from ILL and ESRF has been set up. It is composed of specialists coming from both institutes’ User Offices, Communication Units and Computing Services. They have met regularly with the aim of defining more precisely what “a user single entry point” must be. It was quickly decided to set up a site portal mock-up. The Communication Units and User Offices define the contents; the Computing Services select and set up the adequate tools.

a. Constraints expressed by ILL and ESRF

- Both facilities already have a software application managing their users and experiments. Moreover, both facilities already have their own web site. Even if there are many relationships and collaborations between the two facilities, merging applications and web sites is unrealistic on the short term.
- For the time being, a user having an account at ESRF is identified by an ESRF ID number. If the same user also has an account at ILL, he/she has a different ILL ID number. There are no links between the two IDs. A common portal means a common ID. For obvious reasons we cannot remove local IDs. Consequently, we have to find a way to link the common ID with local IDs.

b. Overview of the foreseen system

The foreseen “single user entry point” system is an umbrella based on a portal. To identify ILL and ESRF users, a unique “site ID” will be provided to everybody. As both facilities already have a local system including a local user ID, a table will link the “site ID” with ILL and/or ESRF IDs. In addition, a field called “European User ID” will be added with a view to be linked with a European-wide user database. The following picture gives an overview of this mechanism.
Other features planned to be provided by the portal are under discussion. A list, information interesting users’ day-to-day life will be included. As mentioned in the introduction, it will be detailed in the deliverable 7.3 planned for November 2009.
8. Specification part 3: ESRF SMIS improvements

8.1 Introduction

The European User Umbrella described in the chapter “Specification part 1” will provide a central point to manage users and affiliations. The Site portal described in the chapter “Specification part 2” will help users coming on site. The specification part 3 focuses on improvements planned to be made in the existing ESRF system. They should be completed in the short term (within two years).

8.2 Technical improvements

The SMIS was first developed by the Institute Laue Langevin in 1979. To manage its proposed workflow, the ESRF copied the ILL software application in 1994. Since then, the ESRF has progressively improved the application by adding new features.

Since 1979, several technologies have been used. Some are no longer supported. Moving software components from a technology to another is time consuming. Resources are often dedicated to developing new components. This is a problem commonly encountered by companies. The work package 9 has been a good opportunity to evaluate new technologies.

Another important evolution over the past fifteen years concerns the software application architecture. In the beginning, the architecture was centralized. The very first software application developed by ILL was centralized on a powerful computer. Then, in the nineties thanks to personal computers, the client-server architecture became the best solution. A significant part of the ESRF SMIS system was developed with this architecture. Then, the internet brought the web architecture. The work package 9 has been a good opportunity to study the web architecture.

8.3 Technical improvements

The new SMIS architecture is now based on three layers:

- The presentation layer interacts with the application user. It communicates with the Business logic layer. The framework STRUTS and the technology JSP have been selected for this layer.
- The business logic layer runs algorithms. It retrieves and stores data using the data storage layer. The Enterprise Java Bean from the company SUN has been selected for this layer.
- The data storage layer manages data. The Relational Database Management System ORACLE has been selected for this layer.
The following picture summarizes the architecture.

Remark: We are currently migrating the whole SMIS system to the new architecture described above. It should be finalized in 2010.
8.4 Adaptations and new features

There are six main improvements planned to be implemented in the short term.

- Connection to the Unified User Umbrella (U³): as described in the specification part 1, the ESRF SMIS system will be linked to the Unified User Umbrella. The existing process of creating SMIS local account will be strongly modified. The process will lead the user to create an account at the (U³) level. Nevertheless, the user will still have the possibility to create an account locally.

- Connection to the site portal: as described in the specification part 2, a portal gathering common information and common applications useful to users coming on site is under construction. The SMIS system will be adapted to be integrated in this portal. SMIS account modifications will be propagated to the site database. All these new features will be described in the deliverable 7.3.

- Joint ILL/ESRF proposals: a joint proposal submission process is planned to be developed. The main goal is to give users the possibility to use ILL and ESRF facilities for an experiment. The proposal will be introduced into ILL and ESRF SMIS systems.

- Extension of the loan pool component: to help people managing the loan of expensive equipment, a software component integrated in the SMIS already exists. Check-in and check-out are recorded manually. An extension in planned to be developed in view of managing the check-in and check-out automatically thanks to embedded WIFI devices or barcode readers.

- Improvement of the proposal review process: the current process to review proposals is a heavy task for the ESRF User Office. The process is partially computerized in the SMIS. The goal is to improve the system with the aim of drastically reducing the time of processing.

- Business Intelligence: for the time being, reports and statistics are developed case by case. Each time, their programming takes several weeks. Business Intelligence tools provide an easy and flexible manner to develop such a software application. Several products are currently evaluated. A selection should be made beginning of 2010. Then, several months will be necessary to install the product.
9. Conclusion

The initial goal of the work package was to specify a new SMIS system, generic enough to be used by all European Facilities. The study shows that partner institutes were not ready to replace their existing systems by a new one on the short term. Nevertheless, several institutes agreed to work on a European portal aiming at providing a central point for users. In addition, the cooperation between ILL and ESRF is progressing well with the goal to provide a site portal to users in the short-term. Finally, the study was a good opportunity for ESRF to evaluate different modern technologies in view of updating its existing system. Even if the initial goal has not been fully reached, a concrete network has been set up between the different European facilities.

The continuation of the three projects (European portal, site portal and SMIS improvement) will provide a coherent infrastructure in the short term. Then, complementary cooperation could be envisaged in order to go further in merging the different European software applications.