PROJECT FINAL REPORT

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Executive Summary

The European Synchrotron Radiation Facility (ESRF), located in Grenoble, France, is a joint facility set up by an intergovernmental convention, supported and shared by 18 European countries and Israel. It operates the most powerful high energy synchrotron light source in Europe and brings together a wide range of disciplines including physics, chemistry and materials science, biology, medicine, geophysics and archaeology. Many industrial applications also benefit from the ESRF's light source and expertise, including pharmaceuticals, cosmetics, petrochemicals and microelectronics. With some 6400 scientific user visits each year, resulting in more than 1500 refereed publications, the ESRF is recognised as one of the world's most innovative and productive synchrotron light sources. This success is also measured by requests for beamtime from the community of users of the ESRF, which consistently exceeds by far the beamtime available.

In order to maintain its leading role and to respond to emerging scientific challenges, the ESRF is planning and now executing an ambitious Upgrade Programme, comprising (i) the extension of the experimental hall to enable the construction of new and upgraded beamlines with largely improved performance and new scientific opportunities, as well as improved infrastructures for the preparation of experiments, (ii) a programme of improvements of the accelerator complex, and (iii) the development of productive science and technology driven partnerships with universities, research institutes and industrial partners. The option for a joint high magnetic field laboratory with the neighbouring Institut Laue-Langevin (ILL) and other European high field laboratories is also being studied. The Upgrade will enable significant progress in fields such as nanoscience and nanotechnology, structural and functional biology, health, environment, energy and transport, information technology, and materials engineering.

Funds of 4.99 M€ were granted by the European Commission within the FP7 Capacities Programme (project acronym ESRFUP) in September 2007 in order to prepare the ESRF Upgrade in its various aspects. Work within ESRFUP comprised the preparation of the legal and technical aspects of the planned building extensions, development of a novel prototype radio-frequency cavity for the storage ring, as well as workshops to discuss the scientific cases for the newly built or upgraded experimental stations and the subsequent preparation of their technical design reports. Roadmaps for detector & data acquisition as well as information technology & data management were developed. Feasibility studies were undertaken for the evolution of the common site infrastructure (ESRF, ILL & EMBL) in terms of harmonised user management and access, and for the possible location of a joint high magnetic field facility. Further actions targeted at increasing the capacity of the ESRF by fostering partnerships for science in specific areas and attracting new member countries and partners from academia and industry.

Description of project context and objectives

The ESRF's 6 GeV storage-ring based synchrotron light source, operational since the early nineties, has been extremely successful in terms of both technical innovation and a very large volume of new and exciting science in fields as diverse as archaeology, biology, chemistry, materials, medicine, palaeontology, physics and many other disciplines, due to the unique combination of X-ray brilliance, source stability, energy spectrum, polarisation properties and overall reliability of the accelerator complex. With some 6400 scientific user visits each year, resulting in more than 1500 refereed publications, the ESRF is recognised as one of the world's most innovative and productive synchrotron light sources. Together with its two neighbouring institutes - the Institut Laue-Langevin (the world leading neutron-beam facility) and the Grenoble outstation of the European Molecular Biology Laboratory - which share the same site, now coined the European Phonon & Neutron Science Campus, the ESRF forms a centre of scientific excellence, unmatched in the world, offering a full range of support services for its visiting researchers.

In order to respond to the new scientific challenges and demands of the user community an upgraded source, new and improved beamlines, and optimised infrastructures are required. This effort has to be embedded in a collaborative network of scientific centres of excellence, not only involving the local partner institutes, but reaching out European-wide. This will enable researchers to exploit a world-wide unique scientific infrastructure and to continue to pursue world-leading research over the next 10 to 20 years. To this end a radical renewal and upgrade programme, requiring a major capital investment, which cannot be financed within the frame of the ESRF's current capital investment budget, is needed. Within this frame the ESRFUP project aims at preparing and catalysing this upgrade programme by a focused effort on the most important aspects:

• Preparation of the legal and technical aspects of the planned building and infrastructure extensions (WP2 and WP12):

Objectives:

- Preparation of the call for tender exercise for the extension of the experimental hall (EX2), selection of the prime contractor, and delivery of the detailed building design report, including the legal building permit file (WP2).

- Elaboration of a partnership proposal for a joint high magnetic field laboratory and report on a prototype magnet design for the proposed facility (WP12).

• Preparation of the scientific cases and establishment of a set of conceptual and technical design reports for the upgrade of the experimental stations(WP4 and WP5).

Objective:

- Obtain feedback and critical input from the user community, develop strategies to cope with the technological challenges, establish a priority list for the beamlines to be upgraded, and to start the preparation of the technical design report for these beamlines.

• <u>Feasibility studies concerning the evolution of the common site infrastructure with the aim to provide efficient (remote) access capabilities (WP7, WP9, WP10) and offer state-of-the-art data handling and archiving procedures (WP11).</u>

<u>Objectives:</u>

- Analysis of the viability of a single point entry system for the ESRF and ILL facilities and specifications for a joint system (WP7).

- Specifications for a new scientific management information system (WP9).

- Definition of a common basis for advanced beamline instrumentation software for the ESRF and concertation with other synchrotron radiation centres in Europe (WP10).

- Assessment of the feasibility to participate in the **E**nable **G**rids for **e**Scienc**e** (EGEE) Grid initiative (WP11).

<u>• Development of know-how and strategies in accelerator and detector technology (WP6 and WP13).</u>

<u>*Objectives:*</u>

- Definition of detector requirements for the future experiments at ESRF and preparation of a pan-European detector development strategy (WP6).

- Design validation of a novel type of radiofrequency cavity to allow the storage ring to operate at a significantly higher current (WP13).

<u>• Enhancement of ESRF's capacity </u>(WP8)

<u>Objectives:</u>

- Analysis of the present and future requirements of the ESRF community and general trends in research with synchrotron.

- Prospection for new member countries to the ESRF and efforts to attract partners who are willing to partly or fully operate an ESRF experimental station.

- Fostering and preparation of partnerships in specific areas of science with academia and industry which shall enable researchers to fully exploit the unique capabilities of the epn campus.

<u>• Dissemination of material describing and advertising the Upgrade (WP3).</u>

<u>*Objective:*</u>

- Provide the governing body, the scientific user community, and the general public with detailed information on all the aspects of the Upgrade.

Beyond these activities, fully or to a large extent funded by the European Commission, additional work within the frame of the ESRF Upgrade needs to be conducted:

• Dissemination of the Purple Book (WP14):

Objective:

The proposed ESRF Upgrade Programme in all its technical, administrative and scientific aspects is laid out in the so called Purple Book (approx. 400 pages) which shall be distributed to the members of the ESRF Council and Advisory Committees, as well as the ESRF user community and policy makers.

• Staff planning and project management (WP15).

Objective:

Study and implementation of a project oriented organisation in parallel to the classical structure by divisions and services.

• Development of know-how and strategies in nanotechnology (WP16 and WP17).

Objectives:

- Development of concepts, hard- and software components, indispensable for experiments involving nano-sized x-ray beams.

- Development of micro- and nano electromechanical systems (MEMS and NEMS) for the conditioning of x-rays.

Main S&T results/foregrounds

ESRFUP started in October 2007, at a stage where the scientific case and the required technological developments were defined and laid out in the so-called "Purple Book". During the first year efforts were concentrated on detailing the scope of the Upgrade in discussions with the user community, and initiating a couple of key activities with the aim to further strengthen the case and convince the stakeholders that the Upgrade is an indispensable step to ensure the world-leading role of the ESRF for the next decade. The key event of ESRFUP was the approval of the ESRF Council on 25 November to officially launch Phase I of the Upgrade (2009 -2016). This marked the official start of the Upgrade, and enabled efforts to be fully deployed as well as to shape the various aspects of the planned improvements. These are laid out in detail below.

<u>Preparation of the legal and technical aspects of the planned building and infrastructure extensions (WP2 and WP12):</u>

In terms of building infrastructure, the extension of the experimental hall (EX2 project) will provide an extra 12,700 square metres to allow the reconstruction and upgrade of approximately half of the public beamlines with greatly improved performance. The extra space will also include room for new support laboratories for sample preparation and characterisation, new offices and facilities. The preparation of the experimental hall extension designs was conducted in 2008. Five companies participated in an international architects' competition. Their offers were thoroughly evaluated by analysis panels of ESRF staff, together with external expert consultants, with expertise in building engineering, stability and safety issues, as well as legal, contractual and financial matters. As an outcome the consortium Sechaud & Bossuyt was awarded an intermediate contract to refine their proposed project according to the evolution of the ESRF's scientific needs, and to reach the ESRF financial targets.

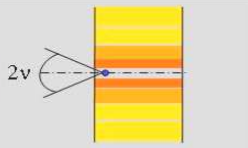
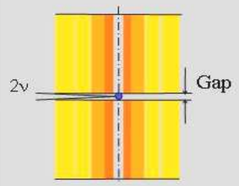
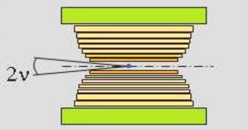
The final contract has been approved and was signed in November 2009. Work on the detailed design studies was launched, and the final design report was submitted at the beginning of October 2010, and subsequently approved by ESRF.

This concluded the tasks to be performed with WP2. Following this, the official work permit was submitted to the local authorities, and construction work on EX2 started in October 2011.

An aerial view of the building extensions as imagined by Sechaud & Bossuyt and view of one of the new laboratory and office buildings

The feasibility study for a High Magnetic Field Laboratory on the joint ESRF/ILL site has revealed that such an installation is possible from a technical point of view. Solutions to bring 40 MW of additional electrical power onto the site as well as the required primary cooling water flow of 4000 m^3/hour, sufficient to dissipate the thermal power generated by the magnets, have been elaborated. Concerning the magnet itself, a horizontal continuous field of up to 38 Tesla could be realised given the results of the feasibility studies to date. Further work focused on the design of a fully split magnet, that is best adapted for X-ray/neutron scattering investigations by offering a vertical magnetic field of up to 30 Tesla. A prototype of a split magnet radial cooling helix, that constitutes the inner resistive part of the fully split magnet, has been designed, successfully realised and tested. In parallel to these technical activities, a partnership proposal was drafted, detailing how the ESRF/ILL High

Magnetic Field Laboratory can collaborate with the four major high field laboratories in Europe - the Grenoble High Magnetic Field Laboratory (GHMFL), the Laboratoire National des Champs Magnétiques Pulsés (LNCMP) in Toulouse, the Hochfeld-Magnetlabor Dresden (HLD) and the High Field Magnet Laboratory (HFML) in Nijmegen - within the framework of a distributed infrastructure.

Magnet	Magnet type		Horizontal Field Magnet Site Detailed in deliverable 12.4.d1	Vertical Field Magnet Site Split Magnet in this deliverable 12.4.d3
	Implementation		Back scattering and absorption magnet site at ESRF	Scattering experiments at ESRF
	polyhelix system	Radial cooling technology		
		Longitudinal cooling technology		
Energy requirements	Electrical Power	Radial cooling technology	24 MW 36 000A max current leads	2 x 17.5 MW 36 000A max current leads
		Longitudinal cooling technology	35 MW 36 000A max current leads	
	Water flow cooling specification	Radial cooling technology	flow rate ≈ 290 l/s Pressure < 40 bar for ΔT = 20°C	flow rate ≈ 2x210 l/s Pressure < 40 bar for ΔT = 20°C
		Longitudinal cooling technology	flow rate ≈ 420l/s Pressure ≈ 25 bar for ΔT = 20°C	
Performance	Magnetic Field	Radial cooling technology	32 T at 35 MW with ν ≈15°	ESRF: 28 T at 35 MW 7 ports with 36° aperture 2x5mm air gap 2x3° take off angle ILL: 30 T at 35 MW 360° aperture 2x5 mm air gap 2x3° take off angle
		Longitudinal cooling technology	40 T at 35 MW with ν ≈ 2°	
	Warm bore diameter	Radial cooling technology	Ø 50mm	Ø 34 mm
		Longitudinal cooling technology	Ø 34 mm	

Magnets suitable for x-ray and neutron scattering as well as x-ray absorption experiments: requirements and expected performance as a result of the design study.

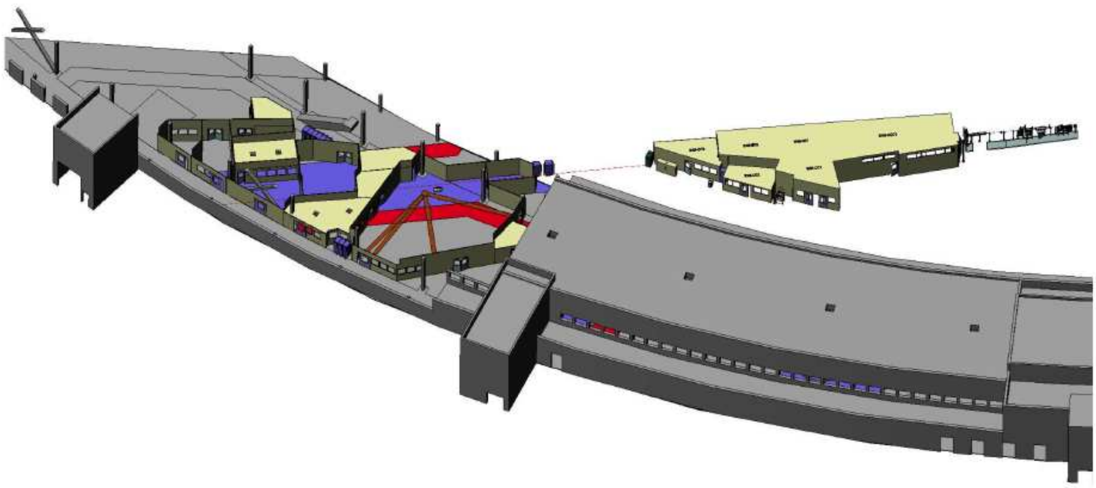
Preparation of the scientific cases and establishment of a set of conceptual and technical design reports for the upgrade of the experimental stations(WP4 and WP5).

Dates	Brainstorming event	Number of participants
	2008	
5 May & 12 September	**UPBL10 Massively Automated Sample Selection Integrated Facility**	24
12 September	**UPBL11 Time resolved and Extreme conditions X-ray Absorption Spectroscopy**	23
15 October	**UPBL7 soft X-ray beamline**	20
12 – 13 November	**UPBL4** & UPBL5 **Nano-Imaging and Nano-Analysis** & Micro-Imaging applications	24
4 December	**UPBL1 Diffraction Imaging for NanoAnalysis**	36
9 – 10 December	**UPBL2 High energy applications in materials science**	16
15 – 16 December	**UPBL9a+b Small angle scattering and structural dynamics**	25
	2009	
13 January	**UPBL6 Inelastic X-ray Scattering**	21
9 – 10 February	UPBL3 Nuclear Resonance scattering	19
23 – 24 February	UPBL8 MINADIF	28

List of ESRFUP WP4 Brainstorming Meetings. The selected eight upgrade beamlines are highlighted in bold.

In order to discuss the ESRF science and technology programme for the next decade as laid out in the reference document, the Purple Book, an Information & Discussion meeting was organised in October 2007. It provided a forum to discuss the scientific aspects of the Upgrade. It gathered about 450 scientists from the user community and ESRF as well as members of the ESRF's Science Advisory Committee and Council. As one of the outcomes, eleven candidate beamlines for a potential major upgrade were identified. To further shape their individual scientific cases and discuss priorities, a series of topical brainstorm sessions were scheduled until February 2009) and discussions took place during the annual ESRF User Meeting and the bi-annual meetings of the Scientific Advisory Committee and Council. These discussions resulted in (i) the selection of eight beamline projects (out of the initially selected eleven candidates) to be rebuilt/upgraded during phase I, (ii) a global overview of the evolution of all experimental stations (the "All Beamline" portfolio containing the conceptual design reports), and (iii) a floor plan, detailing the movement and extension of the beamlines. The series of topical workshops are shown in the figure above; the selected eight Upgrade beamlines are highlighted in bold.

Following the selection of the eight beamline projects (UPBL: UPgrade Beam Lines) significant effort went into the preparation of the technical design reports (TDRs) throughout the duration of the ESRFUP project (and beyond), largely profiting from the possibility to hire extra engineer staff within the project's budget. To date five TDRs have been completed (UPBL4, 6, 7, 10, and 11), and preparations for the UPBL9A (Time-resolved ultra small angle X-ray scattering) and UPBL1 (Diffraction Imaging for nano-Analysis) TDRs started in January 2011. Construction of UPBL10 and UPBL11 has been completed. UPBL10 is well advanced with the commissioning of the beamline components. UPBL11 was officially inaugurated on 10 November 2011, and part of the new facility is open for user operation since 1 September 2011. The UPBL6 project entered the construction phase in autumn 2011.

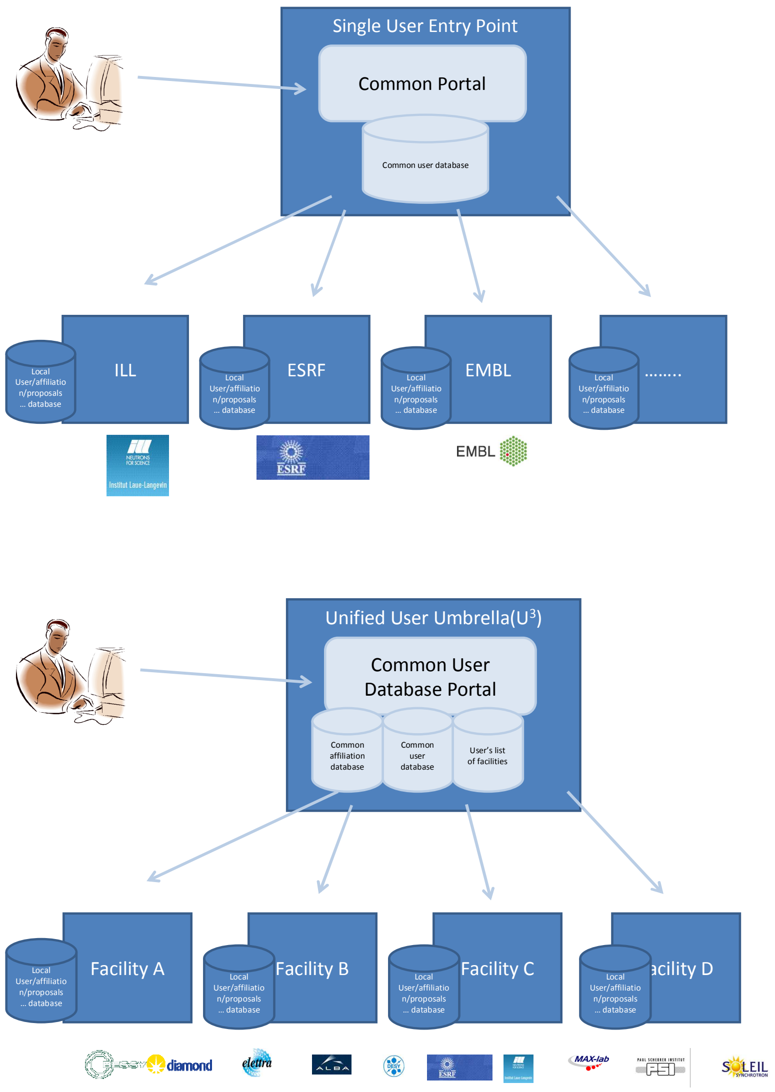


Overall layout for the Soft X-ray beamline UPBL7. The experimental end stations will be hosted in the new Experimental hall EXPH2.

The work performed within WP5 has allowed to streamline and optimise the procedures and the workflow for the preparation and validation of the TDRs. Furthermore, it has facilitated the introduction of a project management structure.

Feasibility studies concerning the evolution of the common site infrastructure with the aim to provide efficient (remote) access capabilities (WP7, WP9, WP10) and offer state-of-the-art data handling and archiving procedures (WP11).

The improved performance of the ESRF will lead to a larger number of users and increasingly demanding requirements in terms of the experiment proposal management, sample tracing, and possible new rules of access. Furthermore, significant progress in terms of data collection, handling and storage has to be made. Several aspects of these challenges were tackled within ESRFUP, in close collaboration with the neighbouring Institut Laue-Langevin (ILL) and other European synchrotron radiation centres.



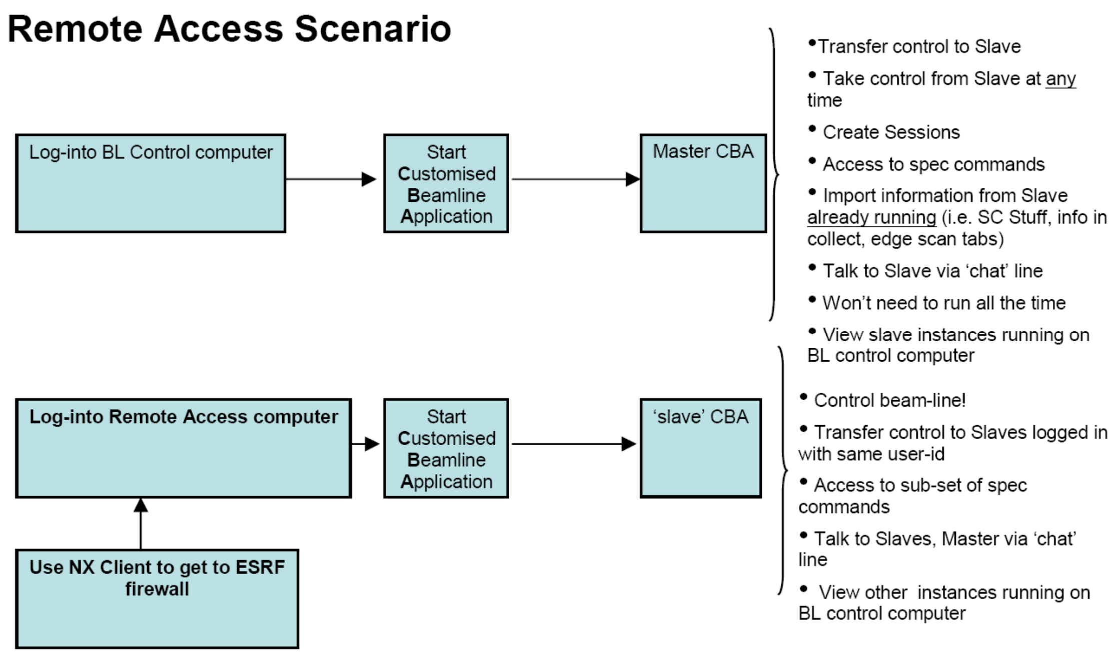
Schematic representation of the single user entry point system to the epn campus site (top) and the proposed common user database portal U^3.

Detailed specifications for a new scientific management information system (SMIS) have been elaborated, including an analysis for a common platform with other research institutes in the European research area. To date the new SMIS system is well advanced, and shall be implemented in 2012. Several other facilities, namely Diamond, ALBA and EMBL Hamburg, showed strong interest, and ESRF provided consultancy for these partners.

To further enhance the visibility and harmonise access to the ESRF and ILL facilities, a common site portal was developed (http:/s/www.epn-campus.eu), and the common ESRF-ILL site, which also hosts the Grenoble outstation of the European Molecular Biology Laboratory, was named European Photon and Neutron Science Campus.

Home page of the epn campus site portal

The viability of a single entry point system for scientific proposals to the ESRF and ILL facilities was studied and a roadmap was laid out specifying which applications could be merged. These comprise a common user authentication and data base, a common proposal and experiment report submission system, as well as common general purpose applications (guest house, restaurant, travel, etc) and common network access.



Schematic representation of the remote access scenario for the structural biology beamlines.

The possibility of running experiments from one's home laboratory is particularly attractive to the large number of users, both academic and industrial, of the macromolecular X-ray diffraction beamlines, and likely other science areas in due course. In this way the user is spared the travel to the ESRF whilst still having full control over the experiment. Organisational and software procedures for remote access to the ESRF have been developed, and first experiments have already been successfully conducted. An integrated beamline software platform, including standardised access to two-dimensional detectors and a generic database for beamline experiment tracking, was designed and implemented. The framework for the standardised access to 2-dimensional detectors; a **L**ibrary for **IM**age **A**cquisition (LIMA) is now utilised as well at Soleil, ALBA and DESY. A workshop on beamline instrumentation software in January 2011 concluded the work. Collaborations on several subjects were formalised, and a users group for integrating detectors was formed in order to foster the sharing of detector integration software.

On the data handling and archiving side, the ESRF took part in the **E**nable **G**rids for **e**Scienc**e** (EGEE) Grid initiative, and has initiated a synchrotron grid with DESY, the Paul Scherrer Institute and SOLEIL as partners. A virtual organisation, called XRAY VO, has been set up and registered in the EGEE. In order to simulate a real Grid setup hardware was procured and installed at the three partner sites with the EGEE gLite software. The test Grid enabled experience to be gained on setting up and managing a Grid site. The study has shown that overall the EGEE Grid is not suited for the case of photon science. The case studies demonstrated that except for a small number of applications (massively parallel programs which are CPU-intensive and require little input or output data) the majority of photon science applications are not suited for highly distributed Grid computing like EGEE. The data intensiveness of photon science applications does not scale to such Grids. Public networks are too slow for transporting large volumes of data to and from storage elements. Most computer software used in photon science which is CPU-intensive and require little data do not need massive parallelisation. They require fast connections between the compute nodes usually based on a protocol called MPI. EGEE Grid provides little support for installing MPI. Furthermore, the photon science communities are organised in a very heterogeneous manner and are much smaller than high energy physics communities. This makes it much more difficult to apply Grid solutions.

The main conclusion therefore is that EGEE grid technology is not the optimum choice for most of the synchrotron science applications. More appropriate solutions comprise the investment in local high performance computing centres and in speeding up the data reduction and analysis by porting programs to the new generation of GPU's and multi-core processors. Remote access to high-power computing centres should be provided, using well-known simple to manage solutions like secure shell.

Development of know-how and strategies in accelerator and detector technology (WP6 and WP13).

In close relation to the beamline developments, detector development strategies and future requirements were elaborated. The development of new X-ray detectors is essential in order to overcome the limitations of current experiments and allow substantial progress in all scientific domains. The preparation work has been focused on defining an overall strategy for detector development at ESRF as well as studying and selecting candidate technologies to be the base of an ESRF proposal for a future joint development programme with other European synchrotron radiation centres, detector development laboratories and detector manufacturers.

A list of proposed development lines that combine technical feasibility and adequacy of ESRF requirements were compiled which shall serve as the starting point for a complete proposal of a detector development strategy to be presented to other facilities in order to pursue a European common action in the field. The overall strategy combines (i) the exploitation of existing know-how and current developments, (ii) beamline specific developments, and (iii) an advanced development programme, focusing on a small number of technologies that are identified as strategic.

The proposed developments are presented in the seven groups below (*a* to *f*) and target two major areas: hybrid pixel detectors that rely on direct detection of incident photons by semiconductor sensors, and indirect detection that make use of X-rays to visible light converters and can eventually use optics for image magnification or demagnification.

a) Semiconductor sensors and interconnection techniques for hybrid pixel detectors.

b) Small-pixel hybrid detectors.

c) Pixel detector readout ASICs with time resolution optimisation.

d) Advanced scintillator materials and structures.

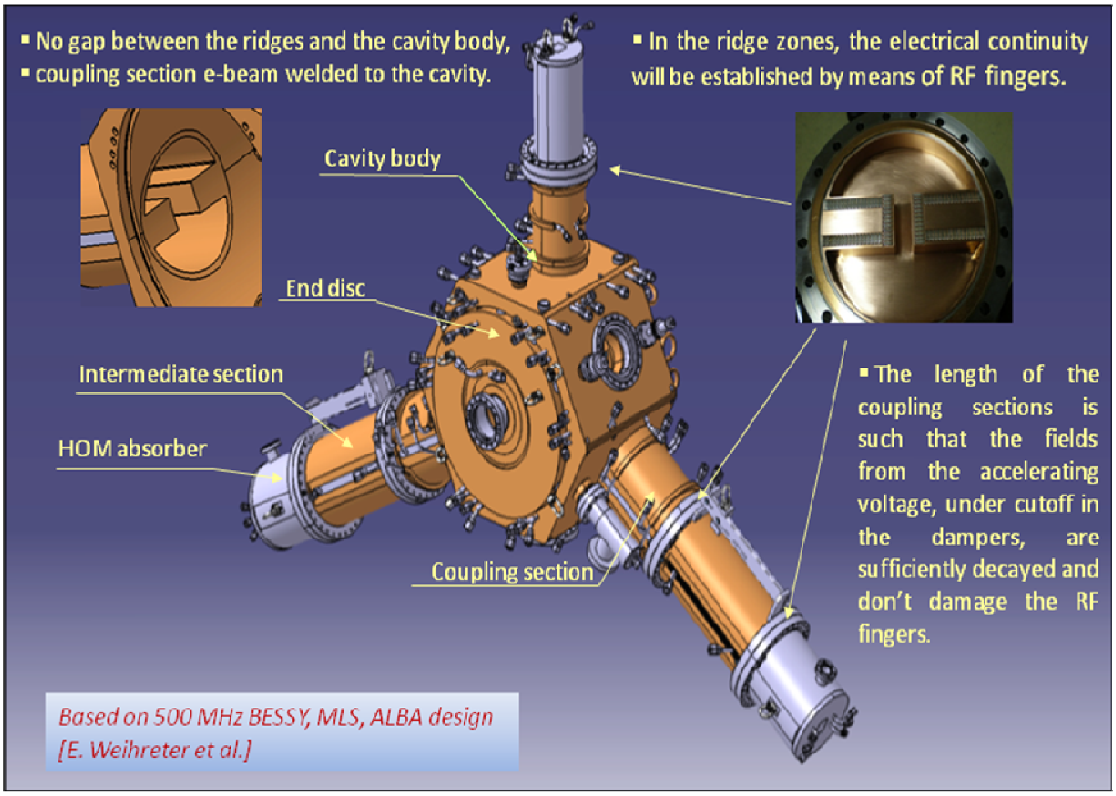
e) Advanced high-quality optical sensors for imaging.

f) High sensitivity high energy scattering/diffraction detectors.

Beyond this a series of collaborations were established with leading synchrotron radiation facilities and other partners, including industry.

The design of a new radio frequency cavity for the storage ring, its manufacture as well as off-line vacuum and power tests were successfully completed. The main results can be summarised as follows:

- A static base pressure of $7.\ 10^{-10}$ mbar was obtained after a few days baking at 130 °C.
- The achieved Higher Order Mode (HOM) damping exceeds the design goal by a factor 2.
- The fundamental accelerating mode remained largely unaffected by the strong HOM damping, and a quality factor, Q_0, of 33800 was achieved, which is at the upper end of the expected 30000 to 35000 range.
- The nominal working point corresponding to an accelerating voltage of V_{acc} = 500 kV was obtained after a few days and as much as 600 kV were reached in a stable and repeatable way with a good vacuum pressure.
- No arcing or overheating of the radio-frequency (RF) fingers was observed.
- No substantial power is coupled from the fundamental accelerating mode to the ferrite tiles which are brazed on the tapered end sections of the ridges in the HOM absorbers.
- As an additional remarkable result beyond the initial scope of this project, an alternative fabrication method was developed during phase 1 of the project and a corresponding 2nd prototype was delivered in July 2011.



The 352.2 MHz HOM damped copper cavity developed at the ESRF in the frame of FP7/ESFRI/ESRFUP/WP13

The fully tested first cavity was installed in the storage ring during the October 2011 shutdown. The successful operation of a vacuum compatible copper prototype confirms the feasibility of such cavities and constitutes a major technological achievement, paving the way for an eventual installation of eighteen such cavities in the storage ring.

<u>Enhancement of ESRF's capacity (WP 8)</u>

Substantial work was dedicated to identify science areas where ESRF member and associate countries might need extra capacity and areas where new partners could be attracted. Furthermore, a European wide synchrotron subscription survey was performed to identify scientific areas of highest interest, and to evaluate the potential for industrial users. The survey included ANKA (Karlsruhe, Germany), BESSY II (Berlin, Germany), DIAMOND Light Source (Harwell, U.K.), DORIS-III / DESY (Hamburg, Germany), ESRF (Grenoble, France), MAX-lab (Lund, Sweden), Swiss Light Source (Villigen, Switzerland), Synchrotron SOLEIL (Gif sur Yvette, France), and as "control" facility the APS (Argonne, USA). The main findings are summarised in the table below.

On the basis of the performed analysis, and in parallel to this, contacts were made with representatives from several countries, most notably Russia, India, South Africa and Brazil. The key event was the signature of a Memorandum of Understanding with the National Research Centre "Kurchatov Institute" (NRC-KI) in June 2011 which opens the way for the Russian Federation to become a full Member of the ESRF.

Science fields	Over-subscribed; growing	Stable-to-growing	Stable		
	Applied materials & engineering; Soft condensed matter; Surfaces and Interfaces	Chemistry; Environment; Electronic & magnetic properties Crystals; Medicine; Cultural heritage	Liquids & disordered systems; Structural biology		
Techniques	**Over-subs / growing**	**Over-subs / stable**	**Balanced / stable**		
	Absorption spectroscopy: electronic; Imaging	Elastic scatt.; Inelastic scattering Single xtal diffraction; Absorption spectrosc.: magnetic	Powder diffraction		
Industrial demand	**High interest / stable**	**Medium interest / growth**	**Medium interest / low growth**	**Low interest / growth**	**Low interest / low growth**
	Pharma; Biotech	Chemical	Electronics	Automotive Energy	Consumer products; Polymers

Analysis of the synchrotron facility subscription survey in terms of scientific fields and techniques as well as demands by industry.

To further strengthen the scientific programme of the ESRF and to complement the X-ray analytical tools by advanced sample preparation/conservation and characterisation facilities, several scientific partnerships were initiated, involving both academia and industry. By nature, this was not a stand-alone effort by the ESRF, but involved the other institutes of the European Photon and Neutron (EPN) Science Campus, most notably the ILL, but also other GIANT[1] partners. The establishment of the Partnership for Soft Condensed Matter was lead by the ILL and received support within the frame of the FP7

[1] The GIANT (Grenoble Innovation for Advanced New Technologies) partnership unites :
European research organisations (ESRF - European Synchrotron Radiation Facility; ILL - Institut Laue-Langevin; EMBL - European Molecular Biology Laboratory),
national research organisations (CEA – Commissariat à l'Energie Atomique et aux Energies Alternatives; CNRS - Centre National de la Recherche Scientifique) and
higher education institutions (UJF - Université Joseph Fourier; G-INP - Grenoble Institut Polytechnique; GEM - Grenoble Ecole de Management)

ILL20/20 project. The Partnership for Extreme Conditions Science is as well a joint effort supported by ESRF and ILL. The attraction of partners with strong emphasis on technology and industrial applications has naturally involved other GIANT partners. These efforts were further facilitated by the economic support from French sources CPER (*Contrat Projets Etat-Région*) to the ESRF and ILL opening new opportunities to develop the international site. The partnership for palaeontology shall provide the required infrastructure from specimen handling and storage to data processing for a user community which has so far not utilised synchrotron x-ray facilities.

Signing the Memorandum of Understanding. Seated from left to right are Mikhail Kovalchuk, Director of the NRC-KI, Jean Moulin, ESRF Council Chairman, and Francesco Sette, ESRF Director General.

The ESRF furthermore facilitated and supported initiatives within the French government programme « Investissements d'avenir » for the development of medium-size scientific installations (EQUIPEX). Two proposals were submitted: HERMeS (High Energy Radiation for Metallurgical Studies) and EcoX (Environmental science using synchrotron X-rays). While funding for EcoX is secured, the decision on the funding for HERMeS is expected by the end of the year.

Dissemination of material describing and advertising the Upgrade (WP3)

Material describing and advertising the planned Upgrade has been disseminated in the form of posters and web page updates to the ESRF governing body, the scientific user community, and the general public**.**

Five press trips were organised to the ESRF, and resulted in several newspaper, television, and other media coverage. Furthermore, three videos on the ESRF Upgrade were produced:

http://www.youtube.com/watch?v=PAQhcz3HPaw (ESRF 2009, English version)
http://www.youtube.com/watch?v=H6SrQEhdkh0 (ESRF 2009, French version)

http://www.youtube.com/watch?v=p4DNQ391fGA (Time on the line, Part 1)
http://www.youtube.com/watch?v=sL5X0_Xsq04 (Time on the line, Part 2)

A dedicated web site was created and regularly updated.

http://www.esrf.fr/, http://www.esrf.fr/AboutUs/Upgrade/

The dissemination activities are detailed in the tables of section 4.2 of the report.

Beyond these activities, fully or to a large extent funded by the European Commission, additional work was performed within the following themes in the frame of the ESRF Upgrade:

Dissemination of the Purple Book (WP14):

The proposed ESRF Upgrade Programme in all its technical, administrative and scientific aspects is laid out in the so called Purple Book (approx. 400 pages). It was produced in 8000 copies and distributed world-wide to the ESRF Council and advisory committees, the ESRF users, other synchrotron light sources, libraries, and policy makers. 1500 copies were sent by post to decision makers and key users, along with a personal letter by the Director General. The Purple book served as a discussion basis for the Upgrade Information & Discussion Meeting which was organised in October 2007, and was distributed at the ESRF User Meeting 2008 as well as at several international conferences.

Staff planning and project management (WP15).

The preparation and implementation of the Upgrade Programme required the establishment of formal procedures for better sharing of resources across the ESRF Divisions and improved consistency and visibility of medium and large-scale projects. As a first step a *Code of Conduct* for project management at the ESRF has been laid down containing all the major definitions and procedures for project management implementation. The structure, function and interaction of all the actors of project management have then been traced. A Project Management Service and a Project Management Board (PCS and PCB) have been put in place with representatives from all the ESRF Divisions for monitoring and regulating the progresses and the cross interactions between the different projects.

The structure of the project itself and of its lifespan has been formally defined as well as guidelines for taking into account necessary changes. The transitions between the different phases of a project (conceptual phase, feasibility phase, execution phase, commissioning and closure) have been formalised with all the necessary requirements. A web-based collaborative project management tool, called ECAPS, was introduced. It offers all the necessary functionalities: planning, archiving, resource allocations, scheduling, etc. The financial analysis and reporting tools have been implemented by upgrading the ESRF Financial Management Information System (FMIS) and redefining the coding for expenditures and projects for cross integration between financial and project tools.

At present the Project Management is integral part of the ESRF culture: the breakeven point represented by a positive return on investment efforts has been reached. In particular the preparation of Technical Design Reports for new and upgraded beamlines (WP5) has largely profited from the introduction of the project management culture at the ESRF. The Instrumentation Service and Development Division (ISDD) is converging towards a structure solely based on ECAPS as management tool.

Development of know-how and strategies in nanotechnology (WP16 and WP17).

As a significant fraction of the Upgrade Programme involves the development of nanoprobe and nano-imaging beamlines, the ESRF management created a Nanotechnology platform in April 2006 in order to cope with the engineering challenges involved. This platform was given two primary objectives and aims at being:

1) A body of technical experts which shall provide assistance and skilled resources for specific instrument developments, interface with industrial suppliers, and perform technical survey and documentation

2) An advisory structure for management on resource management and budget allocations, coordination with other facilities (e.g. on x-ray optics developments), and participation in European networks.

The Nanotechnology platform is composed of working groups, formed around transverse layers involving engineers from the Experiments Division (ED) and Technical Services (TS). Each working group is considered as a reference point for a given engineering expertise and is able to provide technical solutions for approved beamline projects. In particular noteworthy were joint efforts in the field of x-ray optics, where ESRF has coordinated the Joint Research Activity (JRA) workpackage, 'NanoFOX', within the EC-funded FP7 Integrated Infrastructure Initiative (I3), ELISA.

With the creation of the Instrumentation Service and Development Division in April 2009 the concept of the Nanotechnology platform was generalised and extended to other key development areas such as detectors, electronics, software, and advanced analysis. The ISDD provides the technological backbone and expertise for the new portfolio of experimental stations and the improvements of the accelerator complex, and is essential for the success of the ESRF Upgrade.

Potential impact

The ESRF's advanced facilities will substantially strengthen ESRF's central role in stimulating scientific endeavour and economies across Europe by:

- Offering a largely renewed portfolio of experimental stations with often unique capabilities.
- Providing support to academic and industrial research in a complete a way as possible.
- Strengthening existing user communities and attract new communities through scientific partnerships
- Searching for collaborations with industrial partners and fostering synergies with partner institutes on the epn- and GIANT campus.

The new portfolio of experimental stations and the improved infrastructures will attract an even larger user community from Europe and beyond, and offer experimental stations with significantly improved performances in terms of spatial, spectral and temporal resolution as well as throughput. Major impacts can be expected in the following five core areas of applied and fundamental research:

Structural and functional biology and soft matter

Access to synchrotron radiation has revolutionised our understanding of biology, allowing the three-dimensional structure of large biomolecules to be analysed routinely. The impact of these results has extended from an improvement of the basic understanding of Molecular Biology to wealth generation in the European Community. UPBL10 – Massively Automated Sample Selection Integrated Facility – incorporates the three key aspects for a further significant step in scientific productivity, namely high levels of automation of sample handling, automation of X-ray beam delivery and good access to microfocus beamlines that are optimised for Macromolecular Crystallography applications.

The new facility will allow Structural Biologists to tackle ever more ambitious projects, for example more complex membrane proteins and larger macromolecular assemblies. For these samples quality evaluation prior to data collection is essential, as will data collection facilities optimised for the collection of diffraction data from crystals that are very small and/or diffract to low resolution.

Self-assembly is primordial to many fascinating features of soft matter systems. UPBL9a – Small angle scattering – will, amongst others, address how self-assembly brings unique structural and dynamic features which are different from their building blocks. Soft matter self-assembly is also relevant to many nano/biotechnological applications. Although, the equilibrium structure of a large variety of self-assembled systems has been widely investigated, the kinetic pathways of self-assembly remain largely unexplored. Examples include surfactants, block copolymers, and lipid biopolyelectrolytes (e.g. DNA, actin, etc.) complexes.

Nanoscience and nanotechnology

Exploring, manipulating and designing forms of matter at the scale of nanometres is a rapidly burgeoning area, particularly in electronics, medical diagnosis and treatment, and consumer manufacturing. Analytical tools are needed to investigate the structure and behaviour of objects at the nano-scale. New beamlines in which X-ray beams are focused into minute spots about 20 nanometres across will be able to pick out individual biomolecular processes in living cells, or characterise semiconductor structures such as quantum dots at the atomic level. In this respect the upgrade beamlines UPBL1 – Diffraction Imaging for NanoAnalysis, UPBL4 – Nano-imaging and Nano-analysis, and UPBL7 – Soft X-ray Beamline - will play a key role.

Nano-X-ray-fluorescence will elucidate the distribution of trace metals in cellular organelles and nano-X-ray-absorption spectroscopy will identify their chemical state. About one third of all known proteins contain metal co-factors as essential integral structural and catalytic components. These proteins often have regulatory or catalysing functions, e.g., Fe in haemoglobin, Zn in zinc finger proteins as transcription factors in the cell nucleus. In many cases, the trace metals are closely linked to diseases: dysregulation in the homeostatis of one or several metals (e.g., Parkinson, Alzheimer’s, ALS, Friedrich ataxia, Wilson, Menkes, …),. They are also used in therapeutic drugs and diagnostic agents.

Another area is the study of low dimensional systems – “few atom systems”- here the relationship between dimensionality and magnetism is of basic interest while the study of nanomagnets and nanomaterials, in general, is both of fundamental and applied relevance when one considers spintronic applications.

Environmental sciences at the nano-scale include the mineral interfacial reactions at the sub-grain levels: reactivity, bio-availability, and toxicity of (ultra-)fine particles and species adsorbed to surfaces; airborne particles; and colloids in natural systems.

X-ray Imaging

X-rays provide a versatile tool for imaging objects not just in terms of physical structure but also in relation to specific characteristics such as chemical composition and bonding, and magnetic properties. Because X-rays are penetrating, it is possible to build up three-dimensional images of archaeological specimens, machine components and living tissue. Several Upgrade beamlines (UPBL 1, UPBL 2, UPBL4 and UPBL 6) and other experimental stations have or will implement novel and often unique imaging capabilities.

The breadth of new applications comprises archaeology, palaeontology, biological and engineering structures, advanced material and environmental science. Within the frame of the Palaeontology partnership, for example, an end-station will be partly dedicated to the scanning of thousands of fossils at exceptional resolution with the results to be made publicly available.

Thanks to the broad field of new applications in x-ray imaging new user communities will be attracted to the ESRF, thus opening new opportunities in fields of science which so far have not exploited the unique properties of synchrotron X-rays.

Pump-probe experiments and time-resolved diffraction

Recent advances have allowed to track ultra-fast changes in atomic and molecular structures by first triggering the change with a laser (pump) and then analysing it with an X-ray beam (probe) after a given time. UPBL9b – Pump-probe and time resolved experiments – and part of UPBL11 – Time resolved X-ray absorption spectroscopy part – will be able to watch chemical reactions happening for example in industrial catalysts or biological systems on a timescale of less than a billionth of a second.

In fact UPBL11 is the first of the upgrade beamlines which completed large parts of its construction and commissioning. It was officially inaugurated on 10 November 2011, and first test experiments give a flavour of the unique possibilities offered. Important applications lie in the fields of chemistry, life sciences and materials science. Pump-and-probe schemes with time resolutions in the micro- to picosecond range can reveal structural changes in coordination chemistry, proton- coupled electron transfer and electron migration in biology, the decay kinetics of excitons in semiconductors, as well as melting and spin-orbital dynamics in materials science.

Science at extreme conditions

Both academic and industrial researchers often want to know how materials behave under extreme conditions of pressure and temperature, for example, in studies of Earth's and planetary interiors or in a nuclear fusion reactor. The ESRF already provides such world-leading facilities but has further strengthened and enlarged the programme to other x-ray based techniques.

UPBL6 – Inelastic X-ray scattering – will open the possibility of electronic structure studies at high-pressure, coupled to low and high temperatures, and provide access to the properties of low Z materials, for which conventional x-ray techniques such as x-ray absorption and photoemission spectroscopy cannot be applied. The feasibility to perform tomographic studies has been proven recently, showing a tremendous potential in the study of the internal micro-structure of, for example, complex organic materials.

UPBL11 – Extreme conditions X-ray Absorption Spectroscopy – will create new opportunities in the study of the electronic structure of minerals at pressure and temperature conditions of the mantle and core of Earth and other planets, thus attracting the large community of geoscientists. The new facility comprises a set-up employing pulsed magnetic fields up to 30 Tesla. This allows the study of time-dependent magnetic phenomena with a resolution of a few micro-seconds, relevant for the development of magnetic switching devices and other magneto-optical components.

In all these core areas particular attention was given to pave the way for applied science and collaborations with industry, and it is expected that an increasing amount of industrial research will be conducted at the ESRF. Fields of applications include systems relevant to energy research (batteries, fuel and solar cells, hydrogen storage materials, …), catalysis, engineering, electronics and other aspects of advanced technology. Imaging with hard X-rays allows investigation of the liquid fronts in solid-liquid systems of granulates, materials composed of advanced composites and oriented fibres, and storage materials for nuclear waste. Furthermore, the structure and chemical properties of large organic molecules on metal surfaces, and the site distribution of trace impurities e.g. in semiconductors for spintronic applications is of direct interest for technological applications.

The creation of the epn campus as a common site portal for the ESRF and the ILL, and the initiation of several scientific partnerships will strengthen the synergies between the two facilities and, most importantly, outreach to an increasing user community. The largely optimised infrastructures tailored to the needs of the research community in terms of access, accommodation, experiment preparation and control, data reduction and analysis as well as remote access to instruments from home research institutes will boost the productivity of the ESRF and enhance its capacity.

The organisational, technological and scientific developments and advances have been widely disseminated, following legal obligations (e.g. work permits for site infrastructure), publications in specialised (scientific) journals, and presentations to the scientific community. The ESRF organises annual meetings where the user community is informed about the latest developments and advances in science and technology at the ESRF and the status of its Upgrade Programme. These meetings also serve as a platform for exchange, critical input and feedback. Further dissemination activities were mainly conducted within work package 3 and comprised posters, dedicated upgrade web pages, press trips, and three videos. Numerous articles in national and international printed media or on-line journals were triggered. For a full account of the dissemination activities see 4.2.

As ESRFUP was a preparatory phase project several in-depth feasibility and design studies were conducted. Furthermore some innovative hardware and software has been developed, which often serve as a benchmark and example for other research centres and industrial companies throughout Europe. To cite the most important ones (for a full account see Table B2):

Feasibility and design studies

- European-wide user and experiments database
- Software architecture for high speed data acquisition support.
- Integrated beamline software platform
- GRID: Report on operational experiences of the international test bed installation
- Feasibility study of a joint High Magnetic Field Laboratory

Prototypes

- Organisational and software procedures for remote access service
- Technical design reports for synchrotron x-ray experimental stations

- High field magnets for neutron and x-ray experiments
- Prototype of a high-order-mode free radio frequency cavity

The activities of the ESRFUP grant were tightly linked with the activities of the ESRF, which itself generates a significant socio-economic impact at regional, national and European level. In the following, a few examples of a specific impact by the ESRFUP grant are given:

The ESRF contributes to the position of Grenoble as a research-intensive region which facilitates the creation of clusters of good science, talent, technology and start-up companies. Work undertaken under the ESRFUP grant has contributed to the creation of the Technology Platform Grenoble (TP-G), on 10 February 2011, which will pool a wide range of facilities operated by the ESRF, the Institut Laue-Langevin, CNRS and CEA into a single platform for industrial materials characterisation. The decision to set up this joint Platform was largely motivated by the finding from work package 8 of the ESRFUP grant that applied materials and engineering are one of three fields that are generally over subscribed at synchrotrons and are expected to grow. The same holds for soft condensed matter, for which the ESRF and the ILL have set up a similar partnership during the ESRFUP grant.

Procurement and employment are further benefits linked to the activity of a research infrastructure like the ESRF. Under the ESRF grant, new technologies were studied and designed which have led to significant procurements, for example for a new solid-state based RF system for the ESRF storage ring, the procurement value of which exceeds the amount of the grant. In addition, the industrial supplier, a start-up company set-up largely thanks to this procurement, is expected to receive follow-up orders from several new synchrotrons currently being built in China and India.

22 staff were newly employed under time-limited contracts at the ESRF, funded from the ESRFUP grant. Today, after the completion of the contract, nine of these staff continue to work at the ESRF on a regular staff position.

Address of the public website and relevant contact details

http://www.esrf.eu/AboutUs/Upgrade

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