How best to make use of multi-analytical facilities ?

How to fulfil the users requirements?

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OUTLINE

- SOLEIL experience : are there some lessons which we could use to try and improve the efficiency of existing Research Infrastructures ?

- the users needs :
  - friendly use
  - automation
  - data treatment
  - multi analytical platforms/ research institutes
  - use for industry and societal issues

Status

phase I (2002-6) :
construction of the buildings, accelerators and 11 beamlines

the site

the hall

LINAC ready; delivered by THALES ;
a successful technology transfer
Booster ready;
Storage ring : commissioning 31/03/06
Commissioning of the 11 beamlines
from June to December 06
Operation for users : starting in January 07

phase II (2007-9) : construction of 13 beamlines

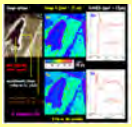
SOLEIL : a novel synchrotron source
for matter and life sciences, and for applications

- An interdisciplinary multi-analytical tool with many different applications for fundamental and applied research :
  physics, chemistry, new materials including nano-materials, earth and environmental sciences, cultural heritage, biology, ...

LUCIA, the first SOLEIL beamline at SLS : X ray micro spectroscopy

An example : the stained glass windows of the gothic cathedrals

Courtesy Farges, Vantelon et al.



✓ particularly true for SOLEIL which is covering a very wide range of photon energy from infrared to moderately hard X rays,

- Initiatives to develop the use for industry (food industry, cosmetics,..) and social issues (cultural heritage, medicine, environment ..)

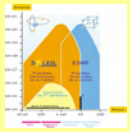
A broad programme with 24 beamlines
answering the users needs

Extensively prepared with and controlled by the future users, French and foreigners

- More than 30 thematic workshops
- Working groups preparing drafts of the scientific and technical cases
- beam-line committees following the construction of the beamlines
- electronic information letters

A broad programme with 24 beamlines
answering the users needs

The users requirements and their satisfactions :



❑ an equilibrium between VUV and soft X-rays on one hand and hard X-rays on the other hand ;

A 2.75 GeV synchrotron covering from 5eV to 15 keV with undulators ;+ Infra Red on BMs

Beamlines : 45% below 1.3 KeV and 55% beyond !

➢ Complementarity with the ESRF as well as with the lower energy facilities (MAX, BESSYII, ELETTRA, ..)

❑ an equilibrium between electron and photon spectroscopy and structural techniques.
11 BLs for spectroscopy and 11 for scattering;

➢ A scientific programme complementary to those of other new sources like Diamond which focuses on x-rays

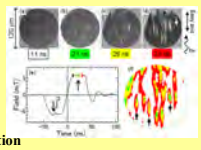
Several specificities

❑ micro beams to investigate complex materials, nano structured ones, for environment, biology,…

✓ A low emittance ring
✓ Optical developments : homogeneous spots in the micron range and below with zone plates
✓ A panel of 5 microscopy and micro-spectroscopy beamlines from infrared to VUV and soft and hard X-ray, + photo- electron microscopy + a proposal for microdiffraction

❑ time resolved experiments

✓ a mode of operation with 8 bunches, 30 ps long
✓ considering 1ps long bunches over a third of the ring and 200 fs ones on a long straight, using bunch rotation
✓ a panel of time resolved experiments in photo electron spectroscopy (magnetism, chemistry), X-ray absorption spectroscopy as well as in diffraction



Domain wall propagation speed (μH = 5.8 mT)
Magnetic tunnel junction on step-bunched Si(111) miscut 6°

Other facilities have other specificities!

A suggestion to make the best use of existing Research Infrastructures :

-To identify specific capabilities in existing Ris and to operate them as European "small" facilities,
- fully open to international access in counterpart of support for their construction and operation
- possibly as a network of several Ris

Examples at SOLEIL : time resolved techniques ; micro-spectroscopies

cultural heritage

SOLEIL, as the other SR facilities, is going to serve a large international scientific community

✓ Probably more than 25 % of foreign users; SOLEIL already open to them in 2007
✓ The SOLEIL company is open to foreign members as well as to international partnerships: CRG's, housing specific equipments, …
Still about 20 beamlines are possible.
✓ Staff scientists : 66% foreigners (transfer of LURE staff excluded

➢ We thank much many European SR facilities helped us a lot, and especially : ESRF, SLS, ELETTRA, BINP: the European community of SR facilities does exist

A strong demand from the Region : SOLEIL as a tool for popularizing science in the broad public, and especially in high schools

The scientific programme

Phase I : 11 BLs opened in January 07 :
1 Infrared village with two lines : one microscopy, one far IR spectroscopy
1 VUV for atomic and molecular physics
2 X-PS :one ARPES +spin; one high flux for time resolved studies (30 picoseconds)
3 XAS : LUCIA Micro XAS ; 2 XAS (energy scanning an dispersive modes)
1 material BL (absorption + diffraction)
3 diffraction including 1PX and 1 small angle scattering

Phase II : 11 BLs opening from 2007 to 2009 :
1 VUV for biology with 3 stations
2 X-PS :one ARPES +spin; one for atomic physics
2 magnetic studies: 1 XMCD, 1 elastic and inelastic scattering +PEEM
5 diffraction including 1PX; 1 high pressure; 2 interfaces; 1 inelastic scattering
1 XAS+ diffraction on radioactive materials
Projects : soft X-ray microscopy
hard X-ray microscopy
micro-diffraction

3rd ECRI web site home page :
"New challenges require an increased international cooperation and sharing of knowledge

The European community of SR facilities already does collaborate much !

There is however still the need to improve efficiency

We believe that the best way to do that is to rely on the users needs

The main users requirement : a user's friendly and efficient operation

☛ control/command and data acquisition

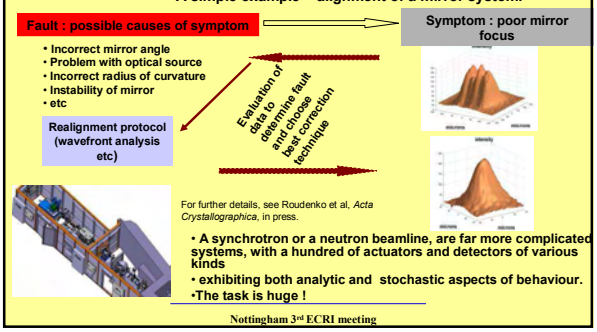
★ Easy and well documented procedures
★ Standardization of the high level of the software running various similar stations.
✓ At SOLEIL, a few groups of beamlines have been identified: scattering, spectroscopy, imaging.
✓ Technically challenging; it needs a lot of resources.

☛ Why not share the work at a multinational level ?

Already some examples :
★ **TANGO: a successful collaboration between several European SR centres for the development of a object oriented software for accelerators as well as for beam-lines : already ESRF, SOLEIL, ELLETTRA, ALBA.**
It should induce a standardization in the software of operation of similar beamlines in these facilities.

The next step : artificial intelligence for diagnostics and control

The task is, given the symptoms, to find the fault and then choose the best corrective action.
A simple example – alignment of a mirror system.



For further details, see Roudenko et al, *Acta Crystallographica*, in press.

• A synchrotron or a neutron beamline, are far more complicated systems, with a hundred of actuators and detectors of various kinds
• exhibiting both analytic and stochastic aspects of behaviour.
•The task is huge !

Already an initiative :the BIOXHIT programme

21 European partners (SR facilities + labs)

Automation from the production of proteins and crystals to the operation of protein crystallography beam-lines and to data collection and analysis.

Programme (web site)

Section 2: Synchrotron technologies chaired by Sean Mcsweeney. ESRF

Based on a radical reconsideration of the beam alignment as a whole, Section 2 aims at the development of beamlines at synchrotron radiation sources, which **allow a complete automatical optical alignment without human intervention**.

Section 3: Beamline endstations and data collection chaired by Colin Nave, CCLRC

The aim of Section 3 is **the automation of crystal mounting to eliminate unnecessary losses of crystals** ...also **allow screening and characterising a large number of crystals** before the final decision for the diffraction data collection is made.

Section 4: Data processing and structure determination chaired by Gerard Bricogne, Global Phasing

Section 4 strives for **integrating the control of data collection with data analysis and with early stages of structure solution to enhance the effectiveness of synchrotron experiments,...to ensure, while an experiment is taking place, that the data being collected have a high probability of leading to a successful structure determination**.

Such an initiative should be extended to other SR fields,

Other RIs would also strongly benefit of it.

Advantages :

- **A potential large saving in operational manpower and a huge increase in reliability.**
- **A strong requirement from industrial users.**
- **Would be of interest for many different types of R Is beyond synchrotron radiation : neutron centres, also electron microscopy, nano-science facilities,……**
- **Technology transfer to industry of stand alone and self-diagnostic systems.**

However, it requires a large effort to characterize the systems and to put in place the machine learning, which is beyond the individual possibilities of most of the European RIs.

A European initiative gathering Research Infrastructures with labs with expertise in artificial intelligence might help much to make a better use of them

Another user's concern : data treatment

☛ **Huge amounts of data are now available from 2D and 3D measurements : PX of course, but also imaging techniques (SR, lasers, NMR …), 3D tomography**
Sophisticated measurements, obtained from several facilities
Data banks with an easy access, to avoid re-measuring, and to insure quality
A large gain in efficiency if data acquisition, treatment and visualisation packages were standardized.

☛ **Data analysis is a bottleneck; improvements are required**
A need raised by SOLEIL future users: how to simultaneously treat imaging data from different techniques : X-ray fluorescence, absorption and diffraction; IR, VUV (lasers and SR) and visible; NMR, as well as other spectroscopic or structural data?
Various I3 programmes could be used, but the requirement is the same for all of them.
A joint initiative?

☛ **Theory not to be forgotten : interpretation is often far behind !**
- Condensed matter : electron, photon (resonant) spectroscopy's, X-ray and neutron inelastic scattering : correlated systems. Already a few networks doing a good job, but still a limited effort.
- Simulation of interaction between any kind of matter and the tremendous fluxes of photons already available in soft X-ray FELs and later on in X FELs : Altarelli talk ?

A major user need : an easy access to other techniques in house or through platforms

☛ **for sample preparation and characterization**
Particularly true for chemistry and biosciences, but also for surface science and material science, including cultural heritage

☛ **use of several techniques is necessary to answer complex questions**
True for all fields, especially true for industrial problems where a unique answer is needed.

★ **In house : possibilities are limited** :
for instance only 4 labs at SOLEIL (chemistry, biology,surfaces, high pressure)

★ **Collaborations with other labs in the surrounding to develop platforms :**
Easy at SOLEIL since it is located close to three major science campus : chemistry backing by the Paris XI University Chemistry Institute; nanostructures preparation / characterization in the MINERVE university platform; a high pressure lab installed on the SOLEIL site and operated by Paris 6 University ; an antenna of INRA (national institute for agronomy), …

Such platforms are important to improve the efficiency of Research Infrastructures

Even more important

Creation of new labs which serve as an interface between the scientific community and the RI: the best way to maximise its research potential

The example of Life Sciences :
complementary strategies at Grenoble with the PSB initiative (ESRF,ILL,IBS) and at SOLEIL with the project of a Centre for Medicament and Molecular Pharmaceutics (4 universities) : crystallography but also cellular and tissues imaging

at RAL : Diamond, ISIS and the Laser and NMR facilities : the Research Complex

Is the national level sufficient ?

An example : nanosciences

In order to accelerate the fundamental research and its transfer to technology, one needs
- state of the art computational methods for designing materials and for optimizing their synthesis process
- advanced synthesis facilities capable to sustain high throughput strategies for inorganic, organic,and bio materials
- advanced analysis facilities including atomic resolution microscopy and methods based on synchrotron radiation micro-spectroscopy and micro-diffraction techniques, and neutron techniques too.
- training facilities
The US have well realized this need : five facilities located close to SR, neutron, laser RIs
There are already many facilities for nanosciences in Europe, but few are connected to RIs, like for instance TASC connected to ELETTRA in Italy.

Questions ?

Do the existing facilities have the required capacities to compete with the US and Asian ones? Do we need to boost them through a European network?
How to ensure complementarities between them?
Interest : to provide access of scientists from countries which do not have such facilities?

Industrial and societal issues requirements

- **Quick access is mandatory**
- **Service should be available any time and without long interruption**
- **Recurrent access is a necessity**

☛ **Despite competition, cooperation is needed between facilities offering a similar service, with exchange of access, and with regular laboratories offering complementary tools.**

- **Full service : from a questionnaire filled up by 40 companies willing to use SOLEIL : 50% want full serviceup to the data analysis and interpretation and 25% a strong assistance**.

This is a real challenge.

To summarize :

- **Cooperation between existing RIs already does exist** (as well as competition) : the example of Synchrotron Radiation centres.
  Similar story for other kinds of facilities.
- **It might be efficiently enhanced by selecting items of broad interest.**
- **Creating new facilities opening new possibilities is a necessity (the road map), but improving the efficiency of the existing ones is another very fruitful one for scientific and industrial use, at a lower cost**
- **A bottom-up strategy starting from the users needs is the most efficient.**
- **A few "cheap"suggestions may be rewarding**: standardization; automation; data treatment; pools of techniques in a network of facilities.
  Certainly many other and better ones !
- **A suggestion : to identify specific capabilities, and to operate them as European "small" RIs, possibly over several facilities, fully open to international access .**