A LIGHT FOR SCIENCE



Pushing the limits of control

Biology: cracking the G-protein code

Industrial evolution: joining the Innovation Union



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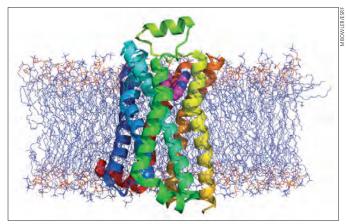
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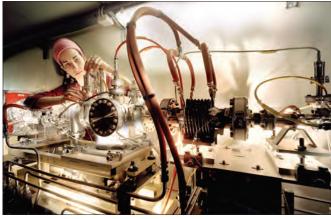
A light for science



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Machine careers: working in the Accelerator and Source Division, p24.



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ESRFnews Control opens up

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When the ESRF entered operation 20 years ago, the computing landscape was very different than it is today. The web had just been born at CERN, e-mail was beginning to take off and object-oriented languages such as C++ were only just starting to become available. The first ESRF control system, TACO, which pioneered object-orientated control systems, was therefore very innovative. It was based on the hardware, operating systems and languages of the late 1980s: Ethernet, VME, OS9 (from Microware, not Apple), Unix and the C language.

Today, OS9 has been replaced by GNU/Linux while VME is being replaced with PCs and embedded intelligent devices connected directly to Ethernet. Unix has been replaced by GNU/Linux and C has been

unify all parts of the system into a single, coherent entity"

"The holy grail of control is to

superseded by C++, Java and Python. The ESRF's control system is now called Tango and it is becoming the *de facto* standard for light sources in Europe as well as being adopted in domains outside the synchrotron world. The US-based control system EPICS is in wider use – about 200 institutes use it compared to some 15 for Tango – but the flexibility of Tango allows it to integrate easily to EPICS, giving users the best of both worlds if needed.

The ESRF decided to develop its own open-source control system, in collaboration with other European institutes, because the object-oriented approach provides an elegant way to manage complexity. It builds a hidden hierarchy of devices representing everything from hardware to complicated data-analysis workflows. Objects can be designed to have the same logical representation as their real-world counterpart: a power supply has current and voltage, whereas such groupings are not possible in flat, non-object-oriented systems.

ICALEPCS in Grenoble

Tango was presented for the first time at the 1999 ICALEPCS conference on accelerator and large-experiment physics control systems in Trieste, Italy. In October this year, the ESRF hosts the 13th ICALEPCS conference, bringing together 450 specialists from the fields of accelerators, telescopes, and large and small physics experiments. It is an excellent chance to strengthen existing collaborations and initiate new ones, since developing software is very human-resource intensive. The standard practice in software development is now "open source", allowing developments and solutions to be shared more easily. Tango is an example of a successful open-source collaboration, but others initiated by the ESRF include LIMA (a framework for 2D detectors), EDNA (for scripting data analyses) and MxCube (for carrying out protein-crystallography experiments). Even software not developed as part of a collaboration is made freely available by the ESRF.

Control systems at the ESRF have to keep pace with increasingly intelligent devices, such as embedded controllers based on flexible hardware devices, called field programmable gate arrays (FPGAs). These have become the standard for developing hardware nowadays, both because they are extremely configurable and because they can cope with very high data flows in digital signal processing thanks to their parallel-processing capabilities. Nowhere at the ESRF is this better illustrated than the beam-orbit correction system, where FPGAs have helped to reduce the vertical emittance to a few pm.

The distinction between software and hardware is being blurred by the massive use of FPGAs, and hardware designers are looking more towards the working practices of software developers. A recent development is the Open Hardware Initiative, spearheaded by CERN, to share FPGA designs for hardware components just as open source does for software.

The holy grail of control is to unify all parts of the system into a single, coherent entity. In the case of the ESRF, that means connecting the hardware to the scientific data-analysis programs and extending Tango's control to the beamlines. This is one of the objectives of the ESRF upgrade, and makes control systems a timely focus for this issue of *ESRFnews*.

Andy Götz, head of the ESRF software group

In brief



Time lapse: the ESRF gears up for a period of flux during shutdown.

Construction brings change

From 5 December the ESRF will enter an extended winter shutdown until 3 May 2012 to allow construction of the experimental hall extension, which will eventually house eight upgraded beamlines. "We will do all our best to maintain normal conditions for users, but they should understand that there will be practical constraints on site," says EX2 project manager Emmanuel Bruas. "It's really a major refurbishment."

Some 10000m³ of earth will be excavated and 1000 tonnes of steel frame erected in the initial heavy-construction period, which will last four months during which site vibrations will be higher than usual. "Apart from perhaps a couple of extreme experiments I don't think users will suffer outside this initial period," says building engineer Paul Mackrill.

The main impact on users, says the EX2 team, will be dayto-day life on site between now and spring 2013. There will be no access to the peripheral road around the experimental hall for at least a year, other than for emergency and service vehicles. Two pedestrian crossings will allow people to reach ID17 and ID19, and parking on the main site will be affected. In short, staff and users can expect to walk a bit further and to watch out for increased traffic on the main entrance road.

"We aim for the highest site safety standards," explains Mackrill. "We are also legally responsible for the safety of people working on the operational part of the site."

The 18-month construction period has been planned with an error margin of just a few days to minimise the effect on users. By the end of 2013, the ESRF will boast brand-new and upgraded beamlines, comfortable new buildings, a new site entrance, all served by a new local tram line. "Then we'll be ready to start the next project," says Bruas.

Christmas comes early for SESAME

The ESRF's reign as the world's sole international light source is soon to end, with the SESAME (Synchrotron-light for Experimental Science and Applications in the Middle East) source under construction in Jordan on track to open in 2015.

To help the project along the way, the Helmholtz-Zentrum Dresden-Rossendorf institute, which operates the German ROBL beamline at the ESRF, has donated the contents of its optics hutch to help establish a new XAS beamline at SESAME. The package includes two large mirrors, a double crystal monochromator plus diagnostic elements, vacuum pumps and control equipment which, if new, could cost around €1.5 m.

"We were upgrading our optics but the old equipment was working fine, so it seemed a waste to send it to the scrapyard," says BM20 head Andreas Scheinost. "I came across the SESAME project a few years ago and found it a fantastic idea to use science to bring people in the Middle East together."

SESAME, which began under the auspices of UNESCO in the late 1990s, is modelled institutionally on CERN, with Bahrain, Cyprus, Egypt, Iran, Israel, Jordan, Pakistan, the



In the post: BM20's optics donation will allow cultural heritage, environmental science and catalysis studies at SESAME.

Palestinian Authority and Turkey current members and 12 other countries as observers. The \$110 m project will be the region's only synchrotron and first international facility.

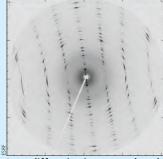
Several sources including SOLEIL and ELETTRA have donated equipment, the most significant being the booster and microtron of Germany's BESSY source and five beamlines from the UK's Daresbury Laboratory. In May, SESAME directors signed a scientific cooperation agreement with Germany's DESY laboratory.

"The original idea was to rebuild BESSY, but it soon became clear that we needed a new storage ring to be a competitive third-generation source," says president of the SESAME council Chris Llewellyn-Smith. "I am very confident it will happen, and 2015 is still possible. There's a good spirit to see this project succeed but the difficulty is funding. We are in a frustrating situation due to the changing political landscape in the region – even organising a meeting is difficult because half of the member countries aren't issuing visas."

Jean Susini, head of the ESRF's Instrumentation Services and Development division, has been appointed to the SESAME training advisory committee, and recently the ESRF produced a SESAME brochure featuring the people behind it. The Spanishoperated beamline BM16 is also considering a donation of redundant equipment. "In the beginning we were accepting most equipment," says Llewellyn-Smith. "Today we are more cautious because we have to assess the costs of adapting it to our machine."

Edible cat litter?

It absorbs more liquid than any other known mineral, is a life saver for cat owners across the western world, and is also relatively rare. Sepiolite, a porous clay used in cat litter, is now giving up its secrets thanks to X-ray and electron diffraction experiments at the ESRF's ID18F and BM25 beamlines, paving the way for synthesis. From different sepiolites samples the team correlated the physical and chemical properties of sepiolite types with their atomic structure.



Laue diffraction image produced by a few fibres of sepiolite.

"The future of sepiolites in the household is outside the litter

box," says lead author Manuel Sanchez del Rio of the ESRF. "Already today, they absorb liquid spillages and odours, and stabilise aqueous products like paints, resins and inks. In synthetic form, they could bind food products and stabilise drugs, extending their shelf life and making sepiolite an edible product." Two Spanish companies specialising in clays – TOLSA and MYTA – are in contact with the team.

Reference

American Mineralogist (in press). DOI: 10.2138/am.2011.3761.

In brief



NRC-KI director Mikhail Kovalchuk.

Russia en route to membership

At a ceremony at the Russian Ministry of Science on 22 June, ESRF directors and members of the NRC Kurchatov Institute (NRC-KI) in Moscow signed a memorandum of understanding concerning Russian participation in the ESRF, with the aim of Russia becoming a full member.

In July, a delegation of ESRF scientists, half of whom were Russian citizens, presented the ESRF's capabilities at the NRC-KI. More than 100 Russian researchers attended at short notice, some having travelled thousands of kilometres.

Russia has two synchrotrons, one at the NRC-KI, but plans to further develop and exploit synchrotron sources. "Russia and its scientists have for over 20 years made important contributions to the ESRF," said ESRF director general Francesco Sette.

Pending full integration, arrangements will be made allowing Russian scientists to conduct experiments at the ESRF. "Russia joining the ESRF would be like opening a door against which people have been knocking for several years," says the ESRF's Alexander Chumakov.

Scan sheds light on our past

The ESRF has helped plug a missing link in our evolutionary past dating from 2 million years ago. Microtomography at ID19 has produced the highest resolution X-ray scan ever made of the brain case of an early human ancestor, shedding light on how the brain evolved during the transition from the genus *Australopithecus* to *Homo*.

"One of our major discoveries is that the shape and form of *Australopithecus sediba*'s brain is not consistent with a model of gradual brain enlargement, which has been hypothesised previously for the transition from *Australopithecus* to *Homo*", says lead author Kristian Carlson from the University of the Witwatersrand in Johannesburg. The brain scan is one of five studies of *A. sediba*'s anatomy carried out by more than 80 scientists published in *Science*.

The brain is long gone having gradually been displaced by a mineral matrix, but X-ray microbeams revealed the imprint of the layers surrounding the brain on the inside of the skull. The "endocast" scan took four days; image reconstruction two weeks; and segmentation – the task of separating, slice by slice, what is bone and what is mineral – a further three months. "The skull really appears as a transitional form," says co-author and ID19 head Paul Tafforeau. "You can



Reconstruction of the skull of *Australopithecus sediba* rendered partially transparent to show the brain endocast.

see general organisation of the lobes, which is possible only with the small [45 micron] pixel scan offered by synchrotrons."

The shape and organisation of the endocast resembles humans more than chimpanzees, yet it is only marginally bigger than a chimpanzee brain. Human brains, by contrast, are about four times bigger than those of chimpanzees. Other parts of *A*. *sediba*'s remains showed similarly advanced features, making it "possibly the best candidate ancestor for our genus," according to co-author Lee Berger from the University of the Witwatersrand, who found the fossil in South Africa in 2009. "We have a lot still to learn about this fossil, for instance from the fine structure of the bone and from the teeth," Tafforeau told *ESRFnews*. "This is only the beginning of the analysis."

Reference

K Carlson *et al.* 2011 *Science* **333** 1402–1407.

Users' corner

Following the 1 September deadline for proposal submission, the next Beam Time Allocation Panel meetings will take place on 27 and 28 October with decisions to be communicated in the first half of December. This year's long winter shutdown, from 5 December until 3 May 2012, means that 60–70% of the usual amount of beam time will be available for allocation in the 2012/I scheduling period.

Work on further upgrade beamline projects will begin during the long shutdown and users are advised to continually check the availability of beamlines for future proposal deadlines at www.esrf.eu/ UsersAndScience/UserGuide/ Applying/beamline-status. The following beamlines were closed to users for the September deadline: ID10A/B/C, ID16 and ID32. The new Soft Interfaces and Coherent Scattering beamline ID10, replacing the ID10A/B/C stations, will open to users in the 2012/I scheduling period and accepted its first proposals at the September deadline. The newly upgraded dispersive EXAFS beamline ID24 also accepted its first proposals at this deadline.

Next proposal submission deadlines: 15 January 2012 for submission of long-term project proposals, and 1 March 2012 for submission of standard proposals, for beam time during the period August 2012 to February 2013.

News from the beamlines • Beamlines ID10A, B and C

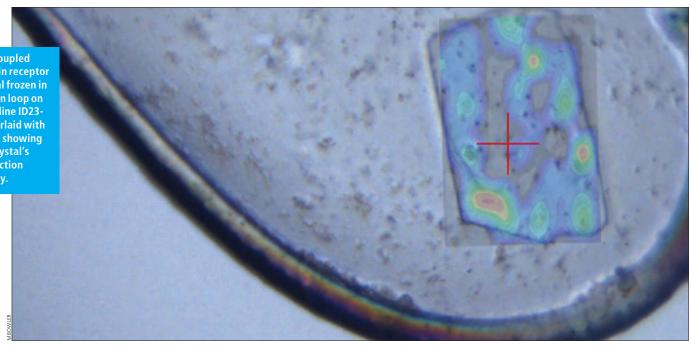
will be rebuilt during the long shutdown as one beamline, ID10, with two experimental hutches working in a time-sharing mode. The new beamline will cover all the activities of the three stations A, B and C.

• Beamline ID16 will move from its current location to ID20 where it will be rebuilt as a fully optimised beamline for inelastic X-ray scattering experiments of electronic excitations. The high-resolution phonon programme will continue on ID28, while BM25B continues to offer capacity for high-energy photoemission experiments.

• The upgraded dispersive EXAFS beamline ID24 will re-open for the 2012/I scheduling period. The new facility features two independent branches; one optimised for a micron-sized focal spot, and the other for tunable focal spot sizes ranging from tens to hundreds of microns. They will operate on a time-shared basis, allowing for more efficient use of beam time.

Feature

A G-coupled protein receptor crystal frozen in a nylon loop on beamline ID23-2, overlaid with a map showing the crystal's diffraction quality.



Cell telephony

ESRF users are cracking the structure of proteins that allow our cells to communicate, revealing important new drug targets.

Do you rely on a shot of coffee to start the day? Thank G-protein coupled receptors (GPCRs) for your kick. These tiny proteins, which are embedded in cellular membranes, spring into action when molecules from inside or outside the body pass by, activating G-proteins inside the cell and triggering a physiological response. Some set off the retina's reaction to light and the nose's response to odours, while others bind to the hormones and neurotransmitters that regulate our moods or affect the strength of our heartbeat.

Over a quarter of all drugs on the market, including treatments for migraine, asthma and heart defects, act on the biochemical pathways stimulated by GPCRs. There are some 800 human GPCRs - half of which are devoted to detecting odours - but only a small proportion of the rest are targeted specifically by current drugs, leaving huge potential for researchers to find suitable activators or inhibitors for the treatment of a wide range of diseases.

Nobel aspirations

While researchers have understood much about the biochemical nature of GPCRs, little was known about how their structure influences the way that the receptor transmits signals through the cell membrane. That situation is changing rapidly thanks to synchrotrons like the APS and, in particular, the ESRF and its automated microfocus beamlines.

"The solution of GPCR structures is ripe for a Nobel prize," says the ESRF's Matt Bowler. "The first structure [of a GPCR that binds to hormones or neurotransmitters] solved four years ago involved a phenomenal amount of work after people had been banging their heads against the wall for over 15 years, but now the structures are coming thick and fast."

The first structural solution of a human GPCR was rhodopsin, the receptor that responds to photons in our retinas, in 2000 - followed by a second structure in a different crystalline arrangement at the ESRF in 2004. But it was 2007 when researchers solved a GPCR that binds to

Inset: crystal structure of activated beta-2 adrenergic receptor $\beta_2 AR$ (red) in complex with G-proteins (green, cyan and yellow).

hormones or neurotransmitters. Using the ESRF's ID13 and ID23-2 microfocus

beamlines, Brian Kobilka's group at Stanford University in the US in collaboration with Gebhard Schertler and colleagues at the MRC Laboratory of Molecular Biology (LMB) in Cambridge, UK, determined the structure of the "beta-two adrenergic receptor" $(\beta_2 AR)$, which is activated by adrenaline and lies behind the

> body's "flight or fight" response by opening the airways in the lungs – making it an important target for β_2 AR agonists used in drugs to treat asthma. "I have a very fond memory of the ESRF," Kobilka told ESRFnews. "Gebhard brought us to the beamline in 2005 to test our

first crystals and again in 2006 and 2007 to collect data that led to the first β₂AR structure.'

The following year, in 2008, the LMB team used ID23-2 to determine the structure of the sister beta receptor, $\beta_1 AR$, which controls the speed of the heart. Knowledge of GPCR structures potentially allows drugs to be designed that bind specifically to only one subtype of receptor, reducing side effects that arise when drugs bind to other receptors.

The struggle for structure

Unlike other proteins, such as haemoglobin solved 60 years ago, membrane proteins are only available in minute quantities and are unstable when removed from their cellular environment, which requires the use of detergents, and they continually undergo conformational "wobbles" even in the absence of an agonist. The key has been to find ways to purify receptors from the membrane so that they are locked in one particular conformation. One approach, developed by the LMB team, is to introduce thermo-stabilising mutations to the receptor, while US researchers have adopted a different approach by using "T4 lysozyme" fusions to reduce the receptor's flexibility. "Fortunately, the two approaches give pretty much the same structure," says Chris Tate, group leader at the LMB

The ESRF's microscopic beam size at ID23-2 has been vital to the recent successes. Structures can now be resolved at 2.5 Å resolution, showing in considerable atomic detail how ligands bind to the receptors.

The beta receptor structures determined in 2007 did not give up all of their secrets because they were all bound to antagonists and were therefore in an inactive state. Earlier this year, however, researchers determined how the beta receptors bind agonists, activating the receptors and relaying this signal to the G-protein inside the cell.

"The big break through of 2011 has been a whole slew of receptor structures that are bound to agonists that initiate intracellular signalling," says Tate, who was part of the team that cracked the β_1 AR's antics at the

"The ESRF made an absolutely key contribution to all of these GPCR structures"

ESRF after a six-month series of visits to ID23-2 last year. The real prize, says Tate, was the structure of the β_2AR in complex with a G-protein determined by Kobilka and collaborators, which shows for the first time in molecular detail how receptors activate G-proteins.

Seven different GPCR structures have now been solved, with many more structures determined of receptors bound to different ligands. "With more than 350 GPCR structures left to solve, there is plenty of room for new players in the field," says Tate. In addition to the all important beta receptors, the ESRF has helped the LMB team solve the structure of the adenosine A_{2A} receptor, which among other things mediates the arousal effect of caffeine.

"The ESRF made an absolutely key contribution to all of these GPCR structures because it was the first [light source] to offer micro-crystallography, which then propagated to other sources," says Schertler who is now at the Paul Scherrer Institute in Switzerland. "Pharmaceutical companies are starting to use this structural information already for drug-design strategies."

The drive for structure determination of GPCRs has so far spun out three biotech companies – Heptares Therapeutics, Receptos and ConfometRx – and many other groups in both industry and academia are now engaged in the GPCR quest. There are parallels with the human genome project, says Bowler. "When people started decoding the genome, people thought it was madness because it would take too long and cost too much, but five years later two teams had developed the techniques and pulled it off."

As for who might receive a telephone call from the Swedish Academy, ESRF users are sure to be among those in the running. But for Kobilka, who insists that many people lie behind the work he directs, the reward has already come. "There's a lot of satisfaction in accomplishing such a major goal," he told *ESRFnews*. "It is a special feeling to have." *Matthew Chalmers*

References

G Lebon *et al.* 2011 *Nature* **474** 521–525. R Moukhametzianov *et al.* 2011 *PNAS* **108** 8228–8232.

S Rasmussen *et al.* 2007 *Nature* **450** 383–387. S Rasmussen *et al.* 2011 *Nature* **469** 175–180. C Riekel *et al.* 2005 *Curr. Opin. Struct. Biol.* **15** 556–562.

D Rosenbaum *et al.* 2007 *Science* **318** 1266–1273.

D Rosenbaum *et al.* 2011 *Nature* **469** 236–240. T Warne *et al.* 2008 *Nature* **454** 486–491.

T Warne et al. 2011 Nature **469** 241–244.

Nobel recognition for structural biology

 1946 Chemistry (J Sumner, half of prize): discovery that enzymes can be crystallised
 1962 Physiology or Medicine (F Crick, J Watson and M Wilkins): molecular structure of nuclear acids and its significance for information transfer in living material
 1962 Chemistry (M Perutz and J Kendrew): structures of globular proteins

• **1964** Chemistry (D Hodgkin): X-ray techniques to solve structures of important biochemical substances

• **1972** Chemistry (C Anfinsen, half of prize): studies of ribonuclease, especially concerning the connection between the amino acid sequence and the biologically active conformation

• 1982 Chemistry (A Klug): crystallographic electron microscopy and the structural elucidation of biologically important nucleic acid-protein complexes

• **1988** Chemistry (J Deisenhofer, R Huber and H Michel): 3D structure of a photosynthetic reaction centre

• **1997** Chemistry (P Boyer and J Walker, half of prize): mechanism underlying adenosine triphosphate synthesis



Winners of the 2009 Nobel Prize in Chemistry.

 2002 Chemistry (J Fenn, K Tanaka and K Wüthrich): methods to identify and analyse structure of biological macromolecules
 2003 Chemistry (P Agre and R MacKinnon): discoveries concerning channels in cell membranes • 2006 Chemistry (R Kornberg): molecular basis of eukaryotic transcription

• 2009 Chemistry (V Ramakrishnan, T Steitz and A Yonath): structure and function of the ribosome

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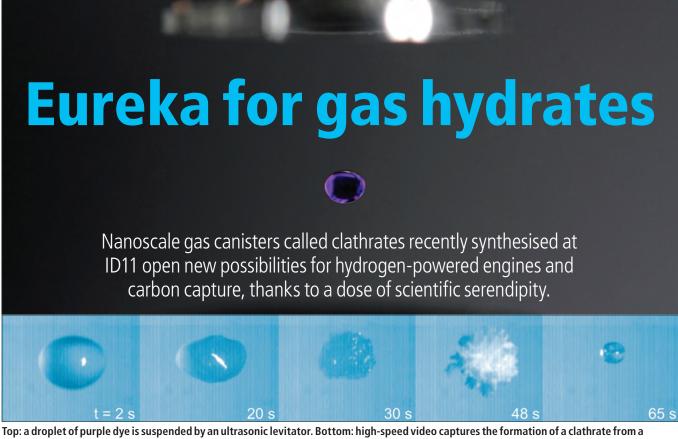


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Top: a droplet of purple dye is suspended by an ultrasonic levitator. Bottom: high-speed video captures the formation of a clathrate from a suspended dichloromethane droplet. Inset below: guest molecules (blue and black) trapped in a cage formed by water molecules.

When engineers tried to stem the flow of oil from the Gulf of Mexico seabed following the 2010 Deepwater Horizon accident, their efforts were hampered by ice-like "mush" that clogged up their equipment. That mush was crystalline cages of water molecules each trapping a molecule of methane, called gas clathrates, which were identified 200 years ago by British chemist Humphry Davy.

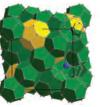
Formed at low temperatures and high pressures, clathrates have been known to block oil pipelines since the 1950s. More recently it has been suggested that some 10¹⁵ kg of carbon is locked up in methane clathrates lying on the ocean floors. That makes clathrates a possible future source of fuel or, less optimistically, a potential environmental disaster if the oceans were to warm up and cause these nanoscale gas canisters to release their guest molecules.

Floating on sound

In April, in conjunction with scientists at the ESRF's ID11 beamline, Franziska Emmerling and a team from Germany's Federal Institute for Materials Research and Testing in Berlin managed to get clathrates to form spontaneously in ambient conditions for the first time. A cubic metre of clathrates contains about 164 m³ of trapped gas, making them ideal candidates for hydrogen and carbon storage materials. "In theory you can pump

out the methane from clathrates on the seabed and simultaneously replace it with CO₂, thereby extracting fuel while getting rid of its combustion products, "Emmerling explained to *ESRFnews*. "But before this could be done on an industrial scale, we have to study how the structures behave."

The team's trick was to use an ultrasonic levitator to suspend small drops of dichloromethane in air, eliminating interactions with container walls. By mixing water into



the droplets, clathrates spontaneously form as the surface cools and dichloromethane evaporates. "This is surprising," says ID11 scientist Jonathan Wright. "Normally you need high pressures and low temperatures to produce these things." The team recorded X-ray diffraction patterns every half second, allowing clathrate nucleation to be monitored at the atomic scale.

Twenty seconds after a drop was injected into the levitator, it began to deform and solidify due to condensation and subsequent freezing of ice on the droplet. After a further 30 s or so it transformed into a white crystalline phase before finally returning to a liquid half a minute or so later.

Although the solid phase of the drop does

not exist for long under ambient conditions, the team was able to stabilise the clathrate by injecting further solvent using a piezo syringe.

Lucky find

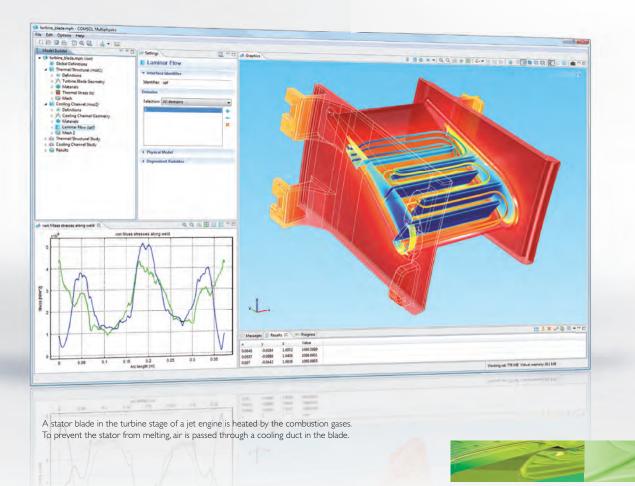
It remains to be seen whether other solvents spontaneously form clathrates under ambient conditions. In fact, it was only by accident that the German team realised dichloromethane could perform the feat. "We were studying polymer formation at the BESSY source last October, and I simply put a drop of solvent into the levitator to make a blank background measurement," says Emmerling. "When I saw reflections I had to check with my PhD student to make sure a crystalline sample hadn't been used by mistake! But I immediately recognised the pattern because, by coincidence, I had studied clathrates for my masters thesis."

The team is planning further ESRF beam time to explore how the speed of nucleation and crystalline structure of clathrates can be tuned, and to investigate the influence of the guest gas molecule on the final structure. "The good thing at the ESRF was that everything turned out perfect and our experiment was completed in less than 10 minutes," says Emmerling. Matthew Chalmers

Reference

2011 Chem. Commun. 47 9369-9371.





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Ahead of the game

The ESRF is tapping into new user communities in anticipation of a Europewide shift to more applied academic research.

Science faces increasing pressure to justify its returns to society, be it spinning out new products or tackling issues such as energy, health and the environment. Funding agencies in many European countries are backing more applied university research, and the European Commission has launched what it dubs the Innovation Union "to ensure that ideas are turned into products and services that create growth and jobs". The strategy will shape research to be funded under the EC's Horizon 2020 Programme (FP8) beginning in 2014.

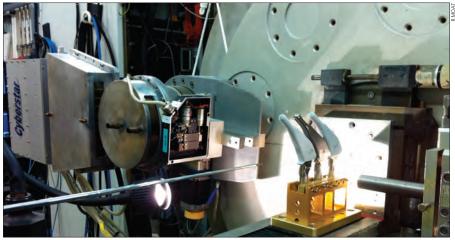
"The world is changing," says ESRF business development manager Ed Mitchell, who is charged with boosting the ESRF's industry profile and liaising with the commercial world. "Fundamental science is a luxury if it's not giving something back to the taxpayer."

A shift in science to more applied and innovation-driven research means new or expanded user communities for the ESRF, namely those close to industry.

Beamlines demystified

The ESRF already has significant industry use. Companies have two modes of access: proprietary, whereby users buy beam time with no obligation to publish, and public access undertaken either alone or in partnership with academic research, for which results must be published in a peer-reviewed journal. The former accounts for about 2% of the ESRF beam time, mostly taken up by large pharmaceutical and biotechnology companies, and amounts to €1.5-2 m per year. Less well known, however, is that an estimated one guarter of the 2000 or so public proposals submitted to the ESRF each year have an industrial component - with an even higher percentage of industry-linked proposals in the fields of structural materials, chemistry and metallurgy.

Industry and innovation-driven research ranges from the highly pragmatic, such as improving manufacturing processes, to fundamental scientific questions that often lead to publications. When a company applies for public rather than propriety access it often seeks an academic partner, for example



Artificial hip joints undergoing recent tests at the ESRF's ID31 beamline.

by funding a PhD position, because it lacks necessary expert knowledge.

The ESRF wants to expand the applied and innovation-driven component of its portfolio by demystifying its beamlines for non-academics. "We should do the blue skies stuff, but do more with industry too," explains Mitchell. "We need to get the message out to companies that the ESRF is not only relevant to universities but that European industry can also expect to benefit from our facilities and expertise."

Docking point

Mitchell and the business development team, which comprises five people including three industrial liaison scientists, are to act as a "docking point" for industrial users, for instance helping them define which beamlines are relevant for their particular problem. "At the start we have to put in some resources, and for that we need people here who do not think in terms of our traditional group-andbeamline structure," says research director Harald Reichert. A planned €6.5 m technology

Industry-linked research at the ESRF

- Saarland University, MPI for Dynamics and Self-Organisation/**BP**:
- Ultrafast tomography at ID15 used to study how an aqueous liquid moves through an oil-filled matrix when it is forced, which may help improve oil recovery rates.
- Leiden University, Eindhoven University of Technology/**Ceram**: Microtomography at ID19 identified link between microstructure and catalytic activity in Ni–Al alloys, helping to optimise their composition (F Devred *et al.* 2011 *Catalysis Today* **163** 13).
- University of Manchester/JRI Limited: Artificial hip joints could last longer thanks to research into how the stresses within titanium alloy joints change over the lifetime of use.

partnership between the ESRF, ILL, CEA and CNRS will help provide necessary resources.

The ESRF is in the process of defining partnerships with specific industrial and academic scientists. The first, in its very early stages, concerns techniques and methodologies for *in-operando* testing of nano- and microelectronics using X-rays, and is being explored in conjunction with the Institute for Semiconductor Physics in Frankfurt and the CEA LETI in Grenoble, both of which have links with numerous smaller companies in the electronics industry which may not yet be aware of the value of synchrotron radiation.

As well as making life on the beamlines easier for users unfamiliar with synchrotrons, the business development team represents the ESRF at trade fairs and is also taking its message directly to companies, such as Lafarge and Janssen. "We are being proactive because we see this shift to applied research coming and we have to be ahead of the game," says Reichert. Matthew Chalmers

 Florida State University and Oxford Superconducting Technology: Tomography at ID15 allows visualisation of troublesome bubbles in superconducting wire during fabrication (F Kametani et al. 2011 Supercond. Sci. Technol. 24 075009).

- University of Manchester/Rolls Royce Aero: Measurements at ID15 and ID31 help to improve safety/longevity of fan blades.
- Montpellier University/TOTAL: Microtomography at ID19 reveals 3D pore structure in limestone before and after injection of CO₂-saturated brine, with implications for carbon sequestration (P Gouze et al. 2011 Journal of Contaminant Hydrology 120 45).
- Toyota: real-time studies of the noble metal components of a vehicle exhaust catalyst reveal structure of the catalyst surface and associated chemical reactions (2008 Angew. Chem Int. Ed. **47** 9303).

CAD diagram of the ESRF with upgrade buildings.

Vacuum system...

944 gauges, pumps and valves with fast diagnostics to help anticipate vacuum deterioration

Magnet system... 1024 magnets that bend, focus and bunch electrons together

Beam orbit correction... passage of electrons generates signals on radiofrequency contacts in 224 beam position monitors, which are processed by field programmable gate arrays (FPGAs) and CPUs to compute the position of the beam in real time and calculate the currents to be applied to 288 corrector magnets

RF cavities... located at six stations around the ring to replenish energy lost by electrons, controlled by Tango to ensure power transferred to the beam at the right time

RF amplifiers... new solid-state amplifiers bring greater reliability than klystrons

Tango... system controlling 200 000 measuring points and actuators necessary for controlling the accelerator complex **Control room...** 10 operator consoles provide user-friendly interface for controlling accelerator complex

History archive... all control parameters since 1993 archived, with each previous year available online for correlation diagnostics

Services... 10 massive flywheels smooth variations in the mains electricity, while air pressure, air conditioning and cooling water are managed by powerline communication networks connected to Tango

Personal safety system... thousands of interlocks hard-wired to work even if the network or the computers are down

Beam shutters...

allow high-power X-rays from storage ring to enter beamlines

Insertion devices... wavelength of X-rays tuned by altering gap of undulator magnets

Beamline alignment... attenuators, monochromators, mirrors, collimators, filters tuned and steered via approximately 10 000 remote-controlled stepper motors

Sample management... samples moved into beam at correct position and angle, synchronised with microsecond precision

Data acquisition and storage... detectors read out data at 100 MB/s (soon to be 1 GB/s) and store it in real time on fast disk arrays

Data analysis... heavy calculations extract meaningful data from thousands of separate images, with increasing online analysis

Experiment sequencer... allows users and staff to adapt the beamline to an experiment

Control choreography

The ESRF's "Tango" is fast becoming a world-leading accelerator and experiment control system, already employed at seven European institutes. Developer *Emmanuel Taurel* describes Tango's next steps.

The ESRF relies on a wide variety of equipment to control its accelerators and drive its experiments. Some pieces are built in-house, others bought in from numerous manufacturers, and each is connected to a computer in its own particular way. Without a unified way to access and control equipment whatever its flavour and guirks, life at the ESRF would be very different: less feedback from equipment means less stable beams, and less automation of experiments means less sleep for users.

The days of linking equipment to a single central computer are long gone. Today, around 150 computers are dedicated to the control of the linac, booster and storage ring while a typical beamline employs three or four computers for experiment control. Staff and users cannot be expected to remember which bit of kit is connected to which computer, so high-level control software must treat a beamline motor or an accelerator power supply equally - even if the motor is driven by a controller that is directly connected on the network and the power supply is connected to a computer using a serial line. The control system must also hide the fact that the equipment is connected to a distributed set of computers

Tango fulfils all of these criteria. The ESRF started Tango at the end of the 1990s to take advantage of the multiple platform provider CORBA and new object-oriented languages, such as Java. We wanted to keep the good points of the initial ESRF control system, TACO, while adding better support for synchronisation, events, asynchronism and device hierarchies. We made sure that Tango interfaced easily with TACO, and made the software freely available under an Open Source licence to encourage collaboration.

This proved to be the right approach because after the first release we were soon joined by SOLEIL, followed by ELETTRA, ALBA, PETRA III, FRM2 and recently MAXlab. These are the official partners who maintain and develop Tango but there are many more Tango users. The system has already been adopted for the experiments at the Laser Mega Joule project in France and by experiments at the FRM II neutron source in Germany. Tango is applicable in any field where a unified protocol for controls is required, even in commercial factories.

Tango may be a mature project, but it is still under constant development. In May the Tango Executive Committee arrived at a roadmap comprising 29 feature requests, including a new event system that will offer a factor of 10 more performance and new data types to facilitate better support

Tango in a nutshell

• Tango keeps the ESRF in step, regulating everything from the air conditioning to the synchronisation of beams with sample stages.

• The control system is distributed across 150 computers comprising VMEs, PCs, process servers and more than 230 Libera FPGAs.

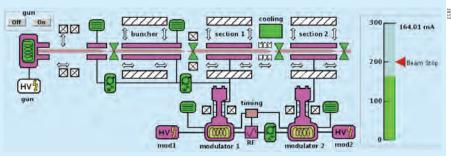
• Equipment is represented hierarchically by Tango in terms of objects (devices), each of which has associated with it certain commands, for example switching a power supply on or off, and attributes, such as position for a motor. sequencers and complex devices like 2D detectors. Historically Tango was used less by the the beamline controls group, but the new upgrade beamlines are controlled mainly by Tango – raising new possibilities for synchronising insertion devices with the beamlines and opening up new kinds of experiment sequences.

We have the right architecture to maintain Tango as a control system par excellence, and there is now a clear way for the system to evolve in the coming months and years. Once implemented, Tango's new features will provide users with higher performance and easier integration of complex devices. In turn, that will result in increased control and better data for all.

• Software specific to the device type is turned into a program called a device server, which runs on the control-system computers.

 Tango comes with tools for configuring and testing the system, storing/retrieving data to/from a database for offline analysis and also offers rich graphical user interfaces with bindings for software such as Matlab, Labview or Igor.

• The control system has to be flexible enough to exploit advances in computing and hardware with minimal interruption to users, which is something akin to changing the wing of a plane during flight.



Tango's graphical user interface keeps the ESRF's linac in check.

Behind the wall

Describing the ESRF control system is a bit like describing a light bulb from the point of view of the French electricity grid, says ESRF software head Andy Götz: as long as it works, users don't worry about it. As electrons journey from their source through the linac, booster and the ESRF storage ring, they do so under the guidance of some 200 000 tunable parameters. Raw electrical pulses deliver instructions to or relay diagnostics from more than 9000 instruments to keep the beam in peak condition, all glued together by Tango.

"When we started in the 1990s, there was no control system to speak of," explains Jean-Michel Chaize, head of the ESRF accelerator control group. "A better control system means a more reliable beam by giving advanced warnings plus it improves beam quality with fast feedbacks, increased focusing and reduced emittance."

Which is the most crucial part of the ESRF control system depends on who you ask. Without detailed diagnostics from the vacuum system for instance, there would be no beam. "Today the ESRF can no longer run, at least not to its normal standards, without the control system," says operation manager Jean-Luc Revol.

The brightness and stability of the ESRF beam relies increasingly on high-level control. Electrons are watched by 224 beam position monitors that capture the weak radio frequency signals produced when the beam passes through, feeding information to the control system which, with the help of fast hardware units called field programmable gate arrays (FPGAs), calculates the necessary orbit correction and sends it to steerer magnets located round the ring.

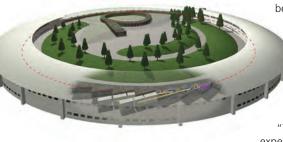
Beam orbit feedback and myriad other systems that keep the electrons on track fall within the domain of "machine" control. But when it comes to photons, and therefore the ESRF's experiments, control passes beyond the storage ring's concrete shielding to the beamlines.

Hidden complexity

An X-ray arriving at a beamline has to be filtered, collimated, tuned and focused to reach the sample, which has to be moved at different positions and angles. The detectors also must be positioned carefully to catch the scattered X-rays, acquiring data as fast as possible before writing them to large disks. The data have to be processed together with the characteristics of the beam to extract what the user is looking for.

The beamlines send requests – say, to alter the gap of an undulator – to the machine

Thousands of interlinked devices, millions of lines of software and good neighbourly relations keep the ESRF's electrons and photons under control.



Dancing in the dark

A power blackout this June caused by an hiccup in the French electricity grid left the ESRF in the dark for 10 minutes, killing the beam and all services, but computers and software were back up and running within a couple of hours. On a separate occasion many years ago, the central computing network hung up completely for almost two hours leaving the control room blind, yet the beam carried on generating photons for users. "It was stable beam at the time," recalls operations manager Laurent Hardy. "It shows just how reliable the physical machine is!" Indeed, the ESRF's magnets and klystrons are among the few systems that can operate independently from Tango. "The whole thing is decoupled as much as possible so that the beam can be kept in the machine without software," says Götz.

control, which has to make sure that such actions do not "pollute" other beamlines by introducing instabilities.

Good communication between the machine and the experiments is therefore vital, as the perfect control of both the accelerators and the beamlines is essential for delivery of useful data to users.

As group leader of the combined machine and experiment control group, Götz says that he is regularly made aware of "the divide". "At one level it's a running joke between colleagues, but sometimes there can be misunderstandings when it comes to the cause of beam quality," he says. "Most ESRF staff have only worked on one side and so can become suspicious about what is happening on the other, but the adoption of Tango on beamlines will ensure sharing of software solutions on both sides."

Chaize likens the accelerator and its beamlines to a medieval castle surrounded by a bustling market: the accelerator has the single objective, planned months or years in advance, of providing a reliable and stable

beam 24 hours a day, whereas beamline control involves many smaller systems that must be flexible to adapt to any unforeseen situation. "In the beamline control world we get very few specifications, and often at the very last minute there are many parallel and successive objectives that can be difficult to marry," says Chaize.

"The accelerator teams should bring their experience in building high-level diagnostics and stable software, while beamline staff should bring adaptability, reactivity and dynamism."

Science in motion

Each beamline is equipped with some 50 motors to drive monochromators, mirrors, sample stages and other components controlled by users. Motion control is one of the hardest control devices to develop, says Götz, because there is non-linear mapping between individual steps of a motor and the final movement of a device handled by way of nine-element arrays. The ESRF has invented its own motion controller, ICEPAP, which has at its core FPGAs capable of being hard-wired with algorithms that transform the reciprocalspace coordinates of, say, a diffraction pattern into tiny accelerations or decelerations of individual motors. FPGAs are fast enough to allow continuous, synchronised motion, directly impacting the efficiency of the experiment because all of the beam time is used for data acquisition.

The challenge for the control across the ESRF is to adapt to the rapid technical improvements in computing and detectors, to expand Tango's reach and to regularly increase the communication speed between hardware and computers and between computers themselves. "Why are storage rings progressing so fast? Because they are using faster feedbacks and better control systems in general," says Chaize. "Unlike a car, where once you have it you don't upgrade the engine to that of a newer model, the ESRF complex is permanently evolving."

Focus on: control systems



Lifting the lid on the ESRF's ID23 beamline.

Crystal control

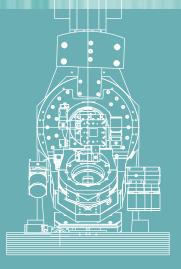
Sophisticated control on the beamlines maximises users' time at the ESRF and opens up scientific studies that otherwise wouldn't be feasible. Take structural biology, where automated sample changing in conjunction with a highly stable micron beam allows hundreds of samples per day to be screened for diffraction quality. "The reliability of the machine control system is a key issue, but the science depends critically on our ability to anticipate flexible control of the optics and the experiments on the beamlines," says Gilles Berruyer, head of the ESRF's beamline control unit.

Serving a large community and responsible for about 45% of ESRF user visits, the structural biology group has made automation a priority – having introduced automatic sample changing in 2003. The number of molecular structures solved worldwide continues to grow rapidly, but with samples becoming bigger and more complex the ESRF is moving toward "secondgeneration" automation with its upgrade beamline MASSIF, where robots loading samples from a dewar will allow thousands of samples to be evaluated per day.

The industrial-like throughput of the structural biology beamlines lends itself to high levels of automation, as do other beamlines such as powder diffraction. Here instrument control provides powerful diagnostics, graphical user interfaces, figures of merit and archiving of configurations. Beamlines where experiments are less "routine" are less suited for automation in part because users have to invent new ways of doing things, so key features of control are scope for evolution, flexibility and fast prototyping.

Remote access is another area where the molecular biology beamlines lead the pack, providing users with the same interface and access that they would enjoy on site at the ESRF. "The science is taking us towards even greater automation and remote access," says Sean McSweeney, head of the ESRF's structural biology group. "But it would be a pity if it gets to the point where scientists stop coming to the ESRF entirely!" Matthew Chalmers

New: Modular Beam Conditioning Unit

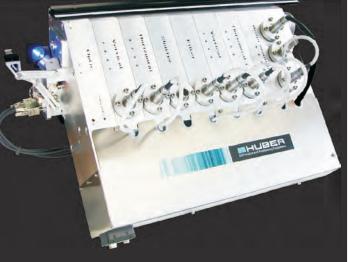


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Field programmable gate arrays are blurring the boundary between software and hardware.

Gone are the days of electronics boards with lots of chips on them. A typical board for scientific applications today consists of one or two chunks of silicon called field programmable gate arrays (FPGAs) – an assembly of logic blocks, which can be configured to perform complex combinational functions. FPGAs comprise memory elements and up to thousands of powerful signal-processing blocks, yet their logic is programmed at the time of power-up similar to a software program, which is loaded into memory at runtime.

"The main benefits of FPGAs are their ability to perform intensive parallel computing and the ease with which their configuration can be perfectly adapted to requirements," says Jean-Marc Koch of the ESRF's power supplies group. "Although it is more difficult to change the functionality of an FPGA than it is a processor, the units can perform very fast operations without the bottleneck of sequential processors, which is vital to keep up with the trend of digitising information as close to the source as possible and with data rates increasing year on year."

The ESRF has adopted FPGAs in major

way for machine control, particularly to stabilise the transverse motion of the beam by adjusting 992 electron bunches individually, turn by turn – a task performed by a single FPGA processing 352 million samples per second. FPGAs are also making their mark on a new beam orbit correction system, with 224 commercial digital

readout units (Libera from iTech) recently installed on the beam position monitors. FPGAs will calculate a correction based on highly accurate position measurements about 10 000 times per second and feed the result to 288 corrector electromagnets.

FPGAs are also helping synchrotrons to manipulate and pre-process data streams generated by state of the art X-ray detectors. "Fast area detectors, such as high-speed CMOS cameras or hybrid pixel devices can produce valuable experimental data at amazing rates – a few GB per second – that are constantly increasing," says Pablo Fajardo, head of the ESRF's detector and electronics group. "The parallel-processing capabilities of FPGAs are essential here to implement a variety of real-time operations at very high speed, from reshuffling bits and applying corrections to transmitting the experimental data to the storage computers."

Increasingly, FPGAs are finding their way into experiment control and synchronisation on the beamlines. The ESRF is implementing its third generation platform for

> beamline control and data acquisition, called DAnCE, based on FPGAs controlled by an embedded CPU running

Linux. More than 100 in-house developed

generic logic and synchronisation modules are used at the ESRF beamlines to exploit the reconfiguration

capabilities of FPGAs. "Traditionally, customising experiment control was limited to swapping electronic modules, changing the cabling and modifying the user software," says Fajardo. "Nowadays, the availability of reconfigurable hardware complements and enhances the possibilities for software customisation with no compromise in performance." Matthew Chalmers

Inset: an FPGA from Xilinx Inc., which invented the technology in 1985.

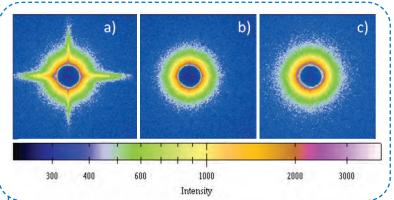
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Images of empty SAXS camera of the D2AM beamline at ESRF, France, collected on a 1.67m SAXS camera and 3mm beamstop, energy set to 17.48keV.

(a) Standard collimation, flux maximized to 3.4e10 ph/s @17.48keV on sample

(b) Same collimation, last anti scatter slits replaced by Xenocs' scatterless slits, same flux

(c) Collimation scheme simplified including Xenocs' scatterless slits allows to increase the flux up to 9.6e10ph/s with same beam focus on detector.



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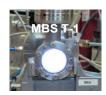
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The ultimate beam

ESRFnews asks accelerator physicist *Laurent Farvacque* – acting director of the accelerator and source division – how far light sources can be pushed.

Has the ESRF beam exceeded expectations?

It's different for different users because some are interested in the total flux, while others who look at small samples want a high brilliance. The maximum beam current went from 100–200 mA in a few years, doubling the radiated power and brilliance, while continuous improvements of insertion devices and beam properties have since increased the brilliance by a factor of more than 100.

Has this surprised you?

From the start we knew that we could do better and better. Being the first thirdgeneration source we had to be conservative initially, whereas new machines today can immediately be more ambitious. There hasn't been a single breakthrough. We do machine studies once per week and have put very high priority on stability and reliability.

How important is the control system?

The beam can survive a short interruption of the control system, but its quality will rapidly degrade. Once you have done everything you can passively, you need active feedback systems. We are relying more on software and control, especially for beam stability, so you gain in performance but are more sensitive to hardware and software failures.

How long could the beam lifetime be?

If you inject a single electron into a perfect machine with no residual gas, it should orbit forever! We're aiming to increase the lifetime by continuing to optimise the filling patterns, vacuum quality and the dynamic aperture.

What's the minimum horizontal emittance?

There is a minimum of about 1 nm based on unrealistic magnet strengths. The ESRF's horizontal emittance was 7 nm in the beginning and went down to 4 nm, but beyond that it is constrained by the machine's layout and energy. We considered major changes to the machine as part of the upgrade and found that while the horizontal emittance could be halved, the gain in brilliance was less than a factor two owing to a broader energy spread. This could not justify the cost and risk.



Laurent Farvacque, ESRF veteran of 25 years, in the ESRF control room.

And the minimum vertical emittance?

Vertically, the emittance could theoretically be close to zero, and the fact that it isn't is down to magnet imperfections. The Libera-based measurement system, which gives us the beam position to a fraction of a micrometre at a sampling rate of 10 Hz, has allowed us to build a more accurate model of the machine, which has enabled a vertical emittance of 4 pm – but a value of 2 pm should be possible.

What is the path to the ultimate beam?

We try to improve our theoretical understanding of the beam behaviour, while also developing better models of the machine and its imperfections. So we rely a lot on the accuracy, speed and signal-tonoise ratio of our diagnostics and benefit from improvements in measuring the beam intensity, position and size.

Why doesn't the ESRF "top-up" the beam?

We have a beam lifetime of around 50 hours, which is much longer than other machines, so if we refill twice a day we get 20% beam loss. The choice of top-up mode must balance the gain in stability resulting from a constant heat load on the equipment versus the additional cost and perturbations due to frequent injections. This is still under consideration.

The ESRF: a victim of its own success?

Other third-generation sources have benefited from the ESRF, but we have also learned from them. The difference between national sources and the ESRF is that we are a high-energy [6 GeV] machine. It was once thought that improved technology would give a 3 GeV machine the performance of a 6 GeV one, but the ESRF also benefited from the technology so this hasn't come to pass.

Will third-generation sources be eclipsed by X-ray-free electron lasers?

Fourth-generation sources like X-FELs provide pulses that are shorter and brighter even than the ultimate storage ring, enabling new experiments. But for many uses, large circular machines will still offer a much higher repetition rate, a better stability and serve more experimental stations simultaneously for a reasonable operating cost.

What will be the "fifth-generation" light source?

The ultimate third-generation machine might be a 2 km-circumference ring with a horizontal emittance of 100 pm – a big improvement on present machines, but with very high costs and massive R&D efforts. Linear machines, referred to as fourth-generation sources, don't suffer the limitations of horizontal emittance and pulse length but they are even larger instruments, which do not completely supersede storage rings. Fifth-generation sources could stem from innovative acceleration methods, such as laser-wakefield acceleration. The beam quality from such systems is a long way from what we have now but it would dramatically reduce the size and cost of the source.

How would you describe your relationship with the machine?

When we restart after a shutdown you feel how the machine responds; you recognise its quirks. In the control room the beam monitor displays something that's really living, and sometimes allows you to detect things that are going on with the beam, which are hard to capture with diagnostics and screens. It's much more interesting than the computer monitors.

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PILATUS detector systems are based on CMOS hybrid-pixel technology and deliver outstanding results in various applications. A wide range of models ensures that a suitable PILATUS detector can be chosen for every measurement.



MYTHEN 1-D detector systems

MYTHEN is a one dimensional silicon strip detector system, which can be combined to form multi-detector arrays covering large angles (MYTHEN 6K).



XBPM Beam Position Monitors

XBPM4 is a 4-quadrant x-ray beam position monitor based on CVD diamond technology, suitable for hard x-ray synchrotron beam lines.





Portrait

'I'm not a synchrotron guy'

Director of the ESRF's Swiss–Norwegian beamlines, **Vladimir Dmitriev**, says that strong collaboration between staff members and users is the key to producing the best science.

The first thing that strikes you when entering Vladimir Dmitriev's office at the ESRF's Swiss– Norwegian beamlines (SNBL) is a large blue sofa next to his desk. Is this the secret, I ask, to his group's extraordinarily high research output: a place for staff to rest between shifts? A therapist's couch, perhaps? "I've never slept here, but postdocs occasionally do," he says.

In fact, one reason for the SNBL's high number of publications – averaging 120 per year, many in high-impact journals, based on around 90 experiments – is Dmitriev's academic background. "I am not a synchrotron guy at all," he says. "I came to the ESRF as a 50-yearold head of crystallography, so I had the mentality of the university professor: publish or perish." Writing a paper is precisely what he would have been doing had *ESRFnews* not dropped by.

Scientific priority

In 1999 Dmitriev was invited to establish an in-house research programme at the ESRF, where he selected SNBL staff on the basis of their scientific as well as technical expertise. "When users come to us they don't always know what is possible here, so our staff members should understand what users want and suggest ideas," he explains. "At the Swiss national source (SLS) the policy is to have more in-house research because that is the basis for quality and productivity."

The SNBL was one of the first CRG beamlines to start operations, in 1994. Initially a predominantly Swiss project with the aim of preparing for the SLS, it evolved into a state-ofthe-art crystallography facility on an equal partnership with Norway. One beamline is devoted to X-ray spectroscopy combined with high-resolution powder diffraction, producing methods and instruments that underpin most high-resolution powder diffractometers used today, and the other is devoted to single



'You'll never work alone" is the motto at the SNBL.

Dmitriev in brief

Born

1949.

Family Married with one son.

Education

University of Rostov-on-Don 1979: PhD thesis "Raman spectra and phase transitions in hydrogen bonded sulphate and selenite crystals".

Work

2004–present: director of the Swiss–Norwegian beamlines at the ESRF
1992–present: University of Rostov-on-Don professor

Interests

Walking in the mountains where he lives; going to the gym two or three times per week; not jogging.

"Ten years ago the CRG and ESRF beamlines were independent communities"

crystal diffraction. Catalysis is a major focus of the SNBL experiments, as are materials for alternative energies.

So what's it like to manage a laboratory within a laboratory?

"One of the benefits is that we are completely independent – we are buying photons from the ESRF and that's it," says Dmitriev, adding that Switzerland is keen to increase its contribution to the SNBL. "But in fact our collaboration with the ESRF is much richer than this. We also report to the ESRF SAC every five years to ensure that our beamlines are technologically and scientifically in step with the level of the ESRF and we publish our financials every two years."

Equal measure

Dmitriev says that he has worked hard to ensure that the CRG beamlines are on an equal footing with the ESRF beamlines. When the former were constructed back in 1994, largely by people from the UK's Daresbury Laboratory, he says there was no unified software or electrical systems or anything common at all – "even the screws were different sizes". Step by step, the CRG beamlines adopted the ESRF's standards. "10 years ago there was a stronger separation between the CRGs and the ESRF beamlines; it was an absolutely independent life of two communities,' recalls Dmitriev. "Now the best CRG beamlines are like family members of the ESRF Experiment Division. We also have very good collaboration with other ESRF beamlines such as ID28, where we can help speed up the search

for critical points in inelastic scattering experiments." As for operating with one proverbial foot in Norway and the other in Switzerland, Dmitriev says that while each country has different scientific traditions, the gap is disappearing. "The Swiss– Norwegian council is totally different to how it was 10 years

ago," he says. "There are no borders between countries, institutes and laboratories any more. Sometimes national ambitions kill the potential of scientific research, whereas facilities such as the ESRF not only bring people from different scientific traditions together but they set standards for other sources. It's one of the most important things I've taken from working at the ESRF." Matthew Chalmers

Careers

Up to speed? Accelerate your career

Team spirit enables the Accelerator and Source Division to give users the best service.

You don't necessarily have to be formally trained in accelerator physics to work in the ESRF's Accelerator and Source Division. "The expertise of the division covers a large variety of jobs, which are united for the development and operation of the source," says operation manager Jean-Luc Revol.

The model of recruiting young staff from various fields to work on the source was set out in the early days of the ESRF by project leader of the ESRF construction, Jean-Louis Laclare. For example, Revol, who has a degree in signal processing and a PhD in applied physics, started working in the RF group 20 years ago. "I could then learn more specifically about accelerator physics and get practical expertise when I started doing machine experiments and tuning," he says. "Today, my job of operation manager touches on everything from infrastructure to machine physics."

Accelerator physics remains a significant part of the division's work, namely the beam dynamics and applications group, because the machine is still evolving despite having been designed and built two decades ago. "There is still a lot to understand about the way particles are accelerated in electromagnetic



An RF cavity for accelerating electrons in the booster synchrotron.

Some 67 people work across 7 groups in the ESRF's machine division:

- Operation: responsible for all aspects of accelerator running, maintenance and development
- Beam dynamics and applications: optimises the source and develops control software
- Diagnostics: develops and maintains instruments for measuring beam parameters
- Front ends: builds and takes care of the equipment at the

fields," says acting division director Laurent Farvacque. "With a single particle, you can exactly calculate its trajectory interface between the X-ray source and the beamlines

- Insertion devices: develops and constructs a wide range of undulators
- Power supplies: responsible for the magnet power supplies and the emergency power supply for the accelerators
- RF and linac: takes care of the linac, high-power RF systems of booster/storage ring and injection extraction magnets

over a period of years, but things get extremely complicated when lots of particles are in a real vacuum tube."

It's unusual for a beamline scientist at the ESRF to cross over to the "machine" division, but the door is not shut to those who have accumulated some technical expertise alongside their science. "When we hire somebody we'd always be looking for a good technical background, such as engineering, plus a PhD in, say, magnetism, RF, diagnostics ideally undertaken at a light source," says Farvacque. The division recently took on a beamline scientist with a PhD in lasers and diagnostics experience.

The ESRF runs a unique scheme whereby staff from all divisions can take part in the operations of the accelerators. Nearly 100 engineers, technicians and administrators spend one or a few shifts per month in the main control room, working as "parttime shift operators" alongside a full-time operator. This scheme, also invented by Laclare, ensures rapid and informal feedback from operation to support groups, and contributes to the record figures for beam reliability and meantime between failures. "The idea of giving our users the best possible support and service is really our shared main objective," says Revol, "and it helps a lot that this responsibility is also shared across the entire ESRF".

Movers and shakers

Director steps down Serge Pérez



ESRF research director Serge Pérez will leave the ESRF at the

end of 2011 for personal reasons. Pérez, who has authored more than 240 papers in the field of glycosciences, joined in 2009 and has been heavily involved in ESRF partnerships as well as phase one of the upgrade.

User success Dorthe Ravnsbæk

The 2011 European Young Researchers' Award went to ESRF user Dorthe Ravnsbæk from the Interdisciplinary Nanoscience Center at Aarhus University in Denmark. Ravnsbæk, who has just completed her PhD, has been a regular visitor to the ESRF's Swiss–Norwegian Beamlines (SNBL) carrying out research into novel metal borohydrides for hydrogen storage applications.

The doctor's doctor Manuela Falanga

The ESRF/ILL campus has a new doctor, Manuela Falanga, who took up her role in July. Dr Falanga, who trained as an occupational physician, was previously the doctor responsible for the care of staff in a hospital in Rome and is also qualified in radiation protection. Falanga told *ESRFnews* that she finds the ESRF's international and scientific environment "very stimulating".

Construction for structure



Some 220 staff from the Insitut de Biologie Structurale

(IBS) in Grenoble are looking forward to moving into a new building on the ESRF/ILL campus. Excavation of the site behind the ESRF guest house is complete and construction of the fivefloor 8000 m² building, due to be ready in 2013, is under way. The move will take IBS researchers closer to the ESRF's Frenchoperated BM30 beamline and to the EMBL, providing "a unique environment for state-of-the-art integrated structural biology in Europe".

Direct advice Christian Vettier

Former ILL science director and leader of the ESRF's magnetic scattering group, Christian Vettier, has taken up a new advisory position to represent the ESRF and ILL on joint issues involving local authorities. It concerns scientific projects on the joint site and specific actions to enhance the visibility of the EPN campus.



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Accelerator Beam Diagnostic Physicist

Argonne National Laboratory invites strong candidates to apply for a staff scientist position in beam instrumentation physics and engineering in the Accelerator Systems Division (ASD) at the Advanced Photon Source (APS).

The APS is the brightest source of high-energy X-rays in the western hemisphere http://www.aps.anl.gov/About/APS_Overview/ and the largest scientific user facility in North America, with more than 3,500 scientists visiting each year to study the structures of materials and processes at the atomic scale. The incumbent will work with a group of physicists, engineers, and technicians and will play a lead role in the design, implementation, commissioning, and analysis of new diagnostic instrumentation associated with the APS upgrade. More information on the APS upgrade is available at http://www.aps.anl.gov/Upgrade/.

Applicants must have a doctorate in a relevant engineering or physical science field and at least six years of subsequent experience or equivalent; considerable knowledge of high-energy particle beam diagnostic and control system design, including beam position monitoring, radio frequency, optical, and x-ray measurement techniques. Considerable knowledge of high-speed data acquisition, analog and digital signal processing, and good knowledge of large-scale control systems such as EPICS and computer programming standards and practices are also highly desirable qualities.

The level at which an applicant will be hire will be dependent on their qualifications and experience.

Interested candidates should apply through the Argonne web site www.anl.gov/jobs for requisition #318088: Physicist, Beam Diagnostics.

Requests for additional information should be addressed to Dr. Alexander Zholents, Director of Accelerator Systems Division via azholents@aps.anl.gov.

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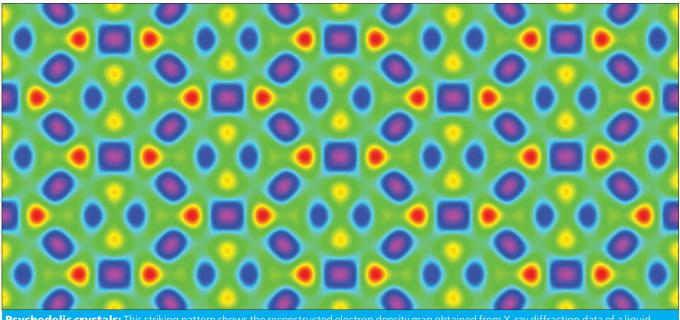
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Beauty of science



Psychedelic crystals: This striking pattern shows the reconstructed electron density map obtained from X-ray diffraction data of a liquid crystal at the ESRF's BM28 beamline – red is the lowest electron density and purple the highest. The map can be explained as a repeated pattern or "tiling" of five different kinds of tiles formed from X-shaped molecules and arranged in complex "honeycomb" phases, with different electron densities resulting from different degrees of mixing among side-groups. The work, by researchers at the University of Sheffield in the UK and the University of Halle-Wittenberg in Germany, reveals the remarkable ability of relatively simple molecules to find the optimum solution to the problem of geometric and compositional frustration – namely by forming periodic structures. This, says the team, will expand the capabilities of "bottom-up" methods of nanopatterning for advanced functional materials. (X Zeng *et al.* 2011 *Science* **331** 1302).

In the corridors

Light up your life



Rainbow: symbol of the IYOL.

The European Physical Society (EPS) has proposed 2015 to be designated International Year of Light, "highlighting to the citizens of the world the importance of light and optical technologies in their lives, for their futures, and for the development of society". The idea – which awaits formal endorsement by the UN -was launched during a workshop at Varenna, Italy, in September titled "Passion for light", at which ESRF director general Francesco Sette delivered a lecture on X-ray vision throughout the decades. According to the EPS, 2015 marks 400 years since the first solarpowered technology, 200 years since Fresnel published his theory of light as a wave, 150 years since Maxwell developed electromagnetism and 50 years since the discovery of the cosmicmicrowave background.

Synchrotron inspiration?

At first sight, Apple appears to be building a third-generation light source. In fact it's its proposed new headquarters in Cupertino, California. At a Cupertino city council meeting held in June, Steve Jobs presented plans for a four-story circular building that will house 12000 people and contain not a single straight piece of glass. "We have a shot at building the best office in the world," said Jobs, who resigned as Apple's CEO in August. "I really do think architecture students will come here to see this." Judging by the city council's response, Apple's new headquarters will face little resistance.



Steve Jobs likened Apple's new offices to a spaceship.

Higgs stirs up Grenoble



No Higgs here: the Alpexpo conference centre in Grenoble.

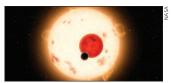
An exciting episode in the halfcentury-long saga concerning the existence of the Higgs boson unfolded in Grenoble in July at the biennial EPS high-energy physics conference. Researchers at CERN's Large Hadron Collider revealed hints that the famous boson - hypothesised to give mass to elementary particles was finally rearing its head in proton-proton collisions beneath the French-Swiss border. But the excitement was short lived: within a month, after more data were collected, the hints looked more like a statistical fluke. By early 2012, however, physicists hope to have written the closing chapter of the Higgs story.

Users' 2012

The plenary session of the 22nd ESRF Users' Meeting will take place on 7 and 8 February 2012 along with two associated workshops: one in magnetic materials under extreme conditions and the other in standing waves and HAXPES. There will also be an MX school in long wavelength phasing.

Binary sunset

Science fiction has become science fact, with the discovery of the first planet to orbit two stars bringing credibility to the twin sunset on the planet "Tatooine" as depicted in the film *Star Wars*. Kepler-16b – a gaseous "circumbinary" planet lying 200 light years from Earth – revealed itself to NASA's Kepler satellite by causing the light from its host stars to dim as it passed.



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It has been designed to achieve an extreme sensitivity range with the best low noise performance for this class of instruments.

