

A LIGHT FOR SCIENCE

ESRF news

Number 57 March 2011

**Seen and heard: reports
from the Users' Meeting**

**Extreme physics: lithium
springs crystal surprises**

**Data-intensive science:
the fourth paradigm**



CVD Diamond in HEP

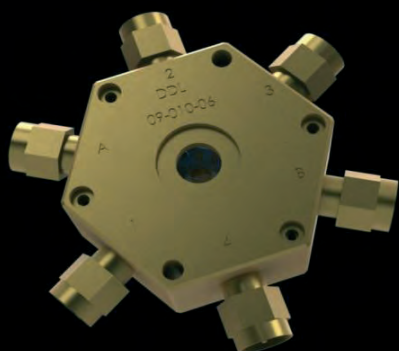
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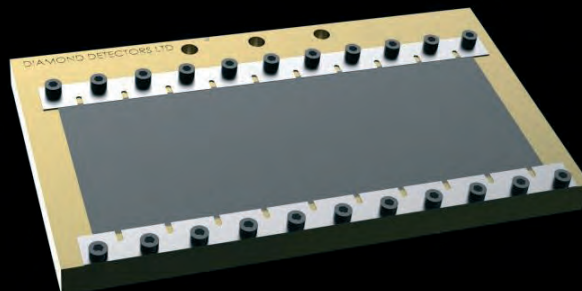
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A light for science



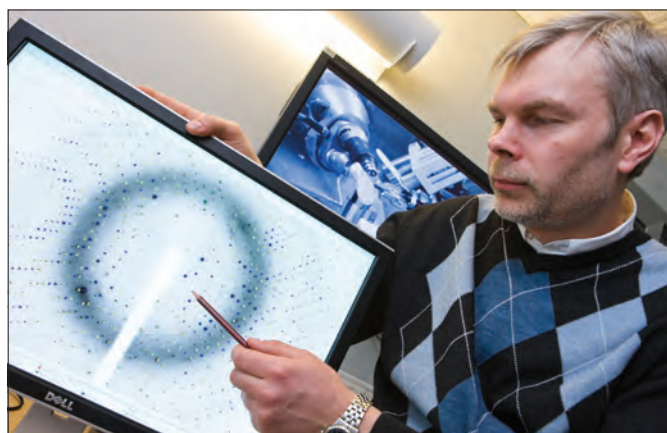
CHANTAL ARGOUÏ

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ISTOCKPHOTOIRVASICK

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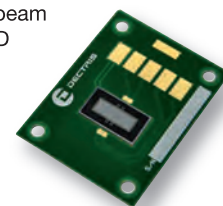
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Letter from the director general: revisions to the Upgrade Programme

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Dear reader,

The ESRF, during the period 2011–2013, will have to manage a 6% reduction of its expenditure capacity compared with the previous medium-term planning that was in place until the end of 2010.

This shortfall will have to be absorbed while minimising any impacts on the high-quality service provided to about 5000 scientists who use the ESRF every year. The main consequence for ESRF users is a process leading to the reduction of the overall amount of beamtime, and to a revision of the Upgrade Programme. The objective is to preserve the main features of the Upgrade Programme – in particular, the eight upgrade beamline projects and the accelerator-complex refurbishment.

This major revision of the ESRF planning in the medium term was initiated at the last Council meeting on 29–30 November 2010 with the adoption of an ad-hoc resolution. It has since then matured into a proposal contemplating the reduction of the ESRF Public Beamlines Portfolio by two beamlines, and the cancellation of approximately one-third of the planned extension of the experimental hall. The decision to close two public beamlines has been reached recently by the ESRF Council following a proposal prepared by the Scientific Advisory Committee (SAC) and management.

Neither an upgrade beamline nor a recently refurbished beamline was considered for cancellation or closure. In narrowing down the analysis to the remaining beamlines, several complementary considerations were taken into account. The final proposal was based almost exclusively on logistical aspects and technical savings strictly connected to the implementation of the Upgrade Programme.

SAC and management jointly proposed to Council the cancellation of the beamline project ID06/ID20 (dedicated to magnetic structure determination) and the closure of beamline ID32 (dedicated to structural and spectroscopic studies using high-energy photoemission and X-ray standing-waves methods). Both measures are envisaged within 2011. Their scientific case will be reconsidered in due course, either when new resources become available or in the context of the Upgrade Programme Phase-II.

The suspension of ID06/ID20 and ID32 from the ESRF Public Beamlines Portfolio was endorsed by the ESRF Council on 11 February. ESRF management has started its implementation, in close consultation with all concerned bodies.

The beamline portfolio of the ESRF will be reconsidered in the future. I am personally engaged to return to a portfolio of 30 public beamlines as soon as possible, to fully respect what has been laid down in the ESRF Convention.

Users' Meeting in the spotlight

The 21st ESRF Users' Meeting has come to a close as I write these lines, and I am very pleased by the quality of the talks, both in the plenary sessions and the satellite workshops, as well as by its attendance. This confirms the support of our users to the ESRF, and highlights the exceptional science that they carry out at our facility. During the first morning session, even the breakout area, to which the Users' Meeting was broadcast from the auditorium, was filled to the last seat. It is a pleasure to see the efforts by the User Organisation crowned by such a success. This issue features a detailed report of the Users' Meeting on pp8–10.

The current *ESRFnews* features articles on the theme of scientific computing, an area in which we are strongly engaged and an activity of growing importance for our users. I wish to thank the writers of the individual contributions and I wish you an enjoyable read.

Francesco Sette, director general

'Excellency' brings a new beamline

The ESRF is a partner in two projects chosen by the French government on 20 January as new infrastructures of "scientific excellency". The projects are among 52 selected from 336 proposals received in response to the €340 m Equipements d'excellence (Equipex) call launched by the Ministry of Higher Education and Research.

The EcoX project, proposed by the University of Grenoble and CNRS, is in line for €4.2 m and foresees a new beamline installed at the ESRF to study the behaviour of metallic elements in biological systems and nanomaterials. The electronic structure and chemical reactivity of metals and metalloids is a major topic in environmental issues, health and toxicity, and chemical engineering, as well as sustainable-energy production.

ThomX is a €12 m project involving seven partners from industry and academia, including Synchrotron Soleil and the ESRF. Its aim is to develop a compact X-ray source with a highly brilliant, directional, monochromatic and tunable beam for applications in medical imaging and therapy, with uses in cultural heritage and industrial technologies too. Following the successful development of a prototype, French company THALES plans to turn this source into a commercial product for hospitals and museums.

Meanwhile, on 16 February a memorandum of understanding was signed by the ILL, the ESRF, the CEA and the CNRS to establish a partnership called PT-G (Plateforme Technologique – Grenoble) dedicated to the characterisation of materials and processes.

Under the terms of the agreement, the four partners will each provide complementary and non-destructive techniques for characterisation and analysis, with the PT-G acting as a focal point for new industrial R&D opportunities.

Key activities will include selection and preparation of samples (with a view to optimising the use of beam time on the instruments) and assistance to industrial users in the processing and interpretation of experimental data.

Diffraction studies shed light on lithium's high-pressure surprises

Being the first metal in the Periodic Table, and with just three electrons, lithium would appear to exhibit simple crystalline structures. But recent experiments at the ESRF have shown that under high pressures lithium has by far the lowest melting point of any elemental metal, and that it undergoes a series of phase changes into surprisingly complex structures.

At ambient conditions, lithium forms rhombohedral crystals which transform to the simplest known crystal structures – face-centred cubic and then body-centred cubic – as the temperature and pressure increase. But in the past few years, intriguing departures from simple metallic behaviour have been observed in more extreme corners of the lithium phase diagram. These include the deviation from simple metal behaviour, a metal to semiconductor transition, and a transition to a superconductor at 17 K.

An international team led by Eugene Gregoryanz from the University of Edinburgh and Michael Hanfland from the ESRF has now used powder and single-crystal high-pressure diffraction techniques at ID09A (along with



DENNIS 'S.K.' COLLECTION

There's more to lithium's crystallographic structure than meets the eye.

single-crystal data collected at the Advanced Photon Source near Chicago) to map out the lithium phase diagram at pressures of up to 130 GPa over a temperature range of 77–300 K. The results show that lithium remains liquid at this high pressure down to temperatures as low as 190 K – by far the lowest melting temperature observed for any material at this pressure. Indeed, the melting point of a material usually rises under pressure.

The work revealed further surprises in lithium's phase diagram. In its solid state above

pressures of 60 GPa, lithium adopts three novel, complex crystal structures with 40, 88 and 24 atoms per unit cell – structures that had not previously been observed in any element, the first two having never been predicted theoretically.

Estimates of the zero-point energy – the intrinsic jitter of particles present even at absolute zero as a result of the uncertainty principle – suggest that quantum effects play a significant role in shaping the lithium phase diagram. The team also speculates that an unusual metallic liquid ground state, which has been predicted but never observed, might be constructed from lithium-rich compounds.

The team had to address several experimental challenges, including handling a diamond anvil cell in a cryostat, ensuring a wide opening angle to allow for single-crystal diffraction, and coping with the high reactivity of lithium – in particular when the element is in the liquid phase.

Reference

C Guillaume *et al.* 2011 Cold melting and solid structures of dense lithium *Nature Physics* doi:10.1038/NPHYS1864.

Winter Atomiades triple success for team ESRF



DAVID BIANCHIN/CANTAL ARGOUÏ

If the tall gold trophy in the ESRF reception looks familiar, it's because the ESRF has won the winter Atomiades for the third time in a row. The ESRF team beat 14 other European laboratories for the overall prize at the La Clusaz ski resort in Haute Savoie on 22–29 January. There were some 260 participants at the event, which was organised by the ESRF and the Association of the Sports Communities of the European Research Institutes. The 12th Winter Atomiades will take place in 2014 in Austria.

Why geobiology runs deeper

Scientists have gained insight into a weird world of life at extreme depths. While temperature is the principal limiting factor for life, pressure plays a major role in the deep marine and terrestrial subsurfaces where large microbial populations do chemistry with the metals that they find there.

The European team, which included three ESRF staff, used X-ray absorption near-edge structure spectroscopy to study *in situ* microbial transformations of metals and metalloids in live bacterial cultures under high hydrostatic pressure.

"This result shows that the metabolic activity of a piezosensitive microbe extends far beyond the pressure range of growth," explains Isabelle Daniel of the Université de Lyon. "Consequently, surface bacteria carried away to depth may impact bio-geochemical cycles in deep water environments."

Reference

A Picardi *et al.* 2011 Monitoring microbial redox transformations of metal and metalloid elements under high pressure using *in situ* X-ray absorption spectroscopy *Geobiology* **9** 196.

Microscopic X-ray beams put art conservation into focus

The intense chrome yellows in Vincent van Gogh's famous *Sunflowers* paintings, which stemmed from the pioneering use of industrial pigments by him and other artists in the late 19th century, could be preserved for future generations thanks to an international study at the ESRF. It has long been known that yellow chrome fades into dark brown with prolonged exposure to sunlight, but microscopic X-ray beams at the ESRF have now revealed the complex chemical reaction responsible.

From a left-over historic paint tube belonging to the Flemish artist Rik Wouters, Koen Janssens of Antwerp University and co-workers obtained a sample of chrome yellow that showed significant darkening after being artificially aged using a UV lamp. By subjecting the sample to X-ray fluorescence and X-ray absorption near-edge spectroscopy, the scientists linked the effect to a reduction of the chromium in the chrome yellow from Cr(VI) to Cr(III).

The affected regions of two van Gogh paintings – *View of*



Microsamples from van Gogh masterpieces were moulded in Plexiglass and placed in the vacuum chamber of the ESRF's X-ray microscope.

Arles with Irises and Bank of the Seine – showed signs of the same reaction in the thin layer where the paint meets the varnish. Because Cr(III) was found to be especially prominent in the presence of barium- and sulphur-containing compounds, the team speculates that the cause of the darkening could be due to van Gogh's technique of blending

white and yellow paint.

The new results suggest that paintings should be shielded as much as possible from ultraviolet and sunlight. "Making this possible has opened the door to a whole new world of discovery for art historians and conservators," says ESRF scientist Marine Cotte, who also works at CNRS/Musée du Louvre.

Van Gogh's decision to use novel bright colours in his paintings is considered a milestone in the history of art, since he chose colours that conveyed mood and emotion rather than employing them realistically. This was completely unheard of at the time, and would not have been possible without major innovations in pigment manufacturing made in the 19th century.

Reference

L Monico *et al.* 2011 Degradation process of lead chromate in paintings by Vincent van Gogh studied by means of synchrotron X-ray spectromicroscopy and related methods *Analytical Chemistry* **83** 1214.

Users' corner

The next Beam Time Allocation Panel meeting to review proposals submitted for the 15 January (long-term projects) and 1 March (standard proposals) deadlines will be held on 28 and 29 April.

The next deadline for standard proposal submission is 1 September. Proposers *must* use the new Experiment Methods template available on the User Guide Web pages, and must ensure that Experiment Reports are submitted for all relevant previous proposals.

The 21st ESRF Users' Meeting and Associated Workshops took place on 7–10 February. For a full report on the Users' Meeting, see pp8–10 in this issue.

Users are reminded to ensure that all new publications

resulting from data collected either entirely or partially at the ESRF are registered in our database via our quick and easy-to-use interface: www.esrf.fr/UsersAndScience/Publications/publication-notification-form.

News from the beamlines

● **The operation contract of the Spanish CRG beamline BM16** will terminate at the end of 2011.

The beamline decommissioning works, originally planned in March, will now begin in September. The beamline will therefore be unavailable for user experiments starting from the 2011/II scheduling period.

● **A new longitudinally curved horizontal mirror** is being commissioned on the CRG beamline **FIP-BM30A**. This mirror is located just before the **MD2** diffractometer. This

optical element will reduce the vertical size of the beam down to ~50 μm, to take advantage of smaller protein crystals. This system should be available for users by April. The mirror and its bender were manufactured by a team at the ESRF. The support was developed in collaboration between FIP, the CNRS/SERAS and the ESRF.

● **A new Pilatus 1M detector** has been installed and is taking data on **BM26B** (DUBBLE). The beamline also has new GDA data-acquisition software.

● **The energy range of the ID21 X-ray spectro-microscope** has been extended up to 9 keV. Co, Ni and Cu K-edges are therefore now accessible for X-ray fluorescence mapping and micro-XANES analyses, still with a submicrometric resolution.

● **The German CRG Rossendorf beamline ROBL on BM20** will be closed for a major optics upgrade in August–September, followed by hot commissioning in October–November. During this period, the beamline will not be available for user experiments.

● **A high-precision diffractometer** coupled to an optical bench has been installed on **ID01** by Huber and commissioned successfully in January. It will allow diffraction from individual nanostructures and functional materials using beam sizes down to 100 nm. Particular attention has been spent on the sample positioning in angular space with precise xyz stages. It has been available to users since February. The smallest beam size obtained so far is 140 nm, and further improvement of the current focusing systems is foreseen in 2011.

The changing landscape of synchrotron science

Exciting science, the upgrade and a new economic climate were the headline themes at the 21st ESRF Users' Meeting held in Grenoble in February. *Matthew Chalmers* reports.

Kicking off the plenary session at this year's ESRF Users' Meeting, Venki Ramakrishnan, who shared the 2009 Nobel Prize in Chemistry for his work on the structure and function of ribosomes, said he owed the ESRF a great debt. "None of the work done by my group over the past 10 years would have been possible without synchrotrons, in particular the ESRF," said Ramakrishnan, who illustrated the twists, turns and grooves of life's building blocks using striking animations.

"Automatic sample changing has really changed our lives, and this has been spearheaded by the ESRF," he added. But the Cambridge-based molecular biologist also said that he hopes the UK's current funding cut will not prevent him from coming to the ESRF in the future. "The UK macromolecular crystallography community is being encouraged to use Diamond, but it's not clear the facility has sufficient capacity to accommodate all our needs without unnecessary delays."

Ramakrishnan was one of 330 participants who congregated under blue skies in Grenoble for three days of lively discussions about ESRF science, with more than 40 presentations given in parallel sessions across seven topics – many as part of dedicated workshops on energy-related materials, time-resolved studies and multiferroics. Single-molecule magnets and the atomic processes taking place on industrial catalysts were among four well attended lectures delivered by invited scientists.

The sheer capacity of ESRF science was highlighted by last year's statistics. Beam time was granted to 1649 experiments in 2010 and the machine's availability was 98.78%, with a record-breaking and "routinely available" vertical emittance of 5 picometres. There were 1723 refereed publications (659 with ESRF authors), bringing to 17 550 the total number of papers published since the ESRF started up in 1994. "I don't know of any other laboratory, in any field, with such an output," said ESRF director general Francesco Sette.

Signalling another productive year, seven papers based on ESRF science appeared in *Nature* and *Science* in the four weeks preceding the Users' Meeting. But it was acknowledged several times during this year's event that the ESRF is moving into a difficult new economic climate. Reductions in contributions from the UK and Italy have



ALL PHOTOS: CHANTAL ARGOUID

"None of the work done by my group over the past 10 years would have been possible without synchrotrons, in particular the ESRF," noted Nobel prize-winning plenary speaker Venki Ramakrishnan.



Gerlind Sulzenbacher (above), chairperson of the Users' Organisation, 2008–2010, coordinated three days of lively presentations and workshops. Sulzenbacher is succeeded as chairperson of the Users' Organisation by Chiara Maurizio (below) from the University of Padova in Italy.



triggered a 6% cut in the budget with respect to 2010 planning, forcing savings of €26 m over the next five years. Sette said that the ESRF had spent a few months preparing for cuts, however, and remains very optimistic about the future.

No compromise

The ESRF's strategy is simple: no compromise on the quality of service to users. Instead, the level of operation will be reduced by 6%. The BM05 X-ray optics and imaging beamline will be closed to external users from 1 March, followed by a reduction from two beamlines to one after the long shut-down in January–April 2012 at the refurbished ID10 soft-condensed-matter complex. These two closures are balanced by new beamlines created within the Upgrade Programme, but the closure of two further insertion-device beamlines was a topic of much discussion at this year's meeting. On 11 February, the ESRF Council formally adopted the cancellation of beamline project ID06/ID20 and closure of ID32 (also see the Editorial, p5).

Meanwhile, the upgrade is in full swing. Work on the experimental hall extension (EX2) will begin this September, while three beamlines are under construction. The UPBL9b project, designed for time-resolved diffraction, has achieved major milestones. As for the TEXAS – Time resolved and Extreme conditions X-ray Absorption Spectroscopy – project (UPBL11), the refurbished BM29 beamline (BM23) opens to users this month while the upgraded ID24 beamlines will open in May next year. The three major components of the "MX village" project (UPBL10) are at various stages. BioSAX will open to users in December this year, while MASSIF (Massively Automated Sample Selection Integration Facility) has experienced a six-month delay in the delivery of lead hutches and will now open in July 2013. Construction of the 100 m-long beamline MAD will begin two years from now, with operation set for May 2014.

Jean Susini, head of the Instrumentation Services and Development division, rattled through some of the numerous advances in optical components, X-ray detectors and beam control systems that are being developed to meet the goals of the Upgrade Programme. They ranged from high-quality diamond crystals to ways of handling 10 GB per second read-outs from the latest

And the winners are...

The **2011 Young Scientist award** was presented to Helen Walker from the electronic structure and magnetism group at ID20 during the Users' Meeting dinner on 8 February. An unexpected outcome of her research into multiferroics using X-rays is the ability of circularly polarised non-resonant X-ray magnetic scattering to measure atomic displacements as small as 10^{-5} nm. "It was a happy coincidence," she recalls. "Applying a magnetic field we found we could induce a displacement and see a big change in scattering, which is something that hadn't been reported by any other technique."

Walker, who has been at the ESRF since 2009, obtained a first-class degree in physical natural sciences from the University of Cambridge, followed by a PhD at University College London and a postdoc at the London Centre for Nanotechnology. "I'm in the middle of a postdoc, but you have to start thinking quite a long time in advance about your next move and recognition like this is always a boost to the CV," Walker told *ESRFnews*. "But to me it's more of an award to ID20 as a whole to recognise the work that's been done there recently." Accordingly,



ALL PHOTOS: CHANTAL ARGOUID

"To me it's more of an award to ID20 as a whole," says Helen Walker, winner of the 2011 Young Scientist award.

Walker said she would fulfil a promise to spend some of the €2000 prize on taking the group to dinner.

The **2011 Best Poster award**, and a cheque for €200, was won by Edinburgh University postgraduate student Thomas Scheler for his poster titled "High-pressure synthesis of platinum hydride". *ESRFnews*



Thomas Scheler receives the Best Poster award for his presentation "High-pressure synthesis of platinum hydride".

would also like to congratulate ESRF thesis student Max Langer for producing the most digitally enhanced poster (with built-in screen showing X-ray microtomography of bone), and artist Céline Berger for producing the most unusual poster: a video project to investigate how scientists perceive time during shifts on the ESRF beamlines.

2D detectors, and also demonstrated the phenomenal accuracy of modelling. The ESRF faces what Susini calls "the Lego challenge": finding the most cost-effective way to balance commercial versus in-house components to meet the demands of highly specialised beamlines surrounded by instruments that push current technology to its limit.

In effect, remarked Susini, users have a new ESRF on their hands: an enhanced machine with more than 20 renewed end stations, a new building infrastructure and data centre, plus new organisation, practices and enabling technologies. "When I think of the upgrade, I think of Janus," said Susini. "Looking to the past we have the capital of 20 years' experience, while looking to the future we have new detector technologies, automation and data management to deal with. With the new ESRF also comes a new economic and rapidly evolving international context."

Changing landscape

Tighter financial conditions are being experienced throughout European and US science, but the synchrotron community also has to grapple with an increasing number of facilities: in Europe there are currently 13 operational synchrotrons of the highest performance compared to just one when the ESRF started up. "One question that we need to answer is whether Europe has too many light sources?" Sette explained to *ESRFnews* during the meeting's poster session. "I am convinced that there is an increasing need for synchrotron science in both fundamental and applied research. Therefore the answer is no. However, it is mandatory today to increase the

coordination among all of these sources to fully exploit the investment."

Sette said that in addition to highlighting the numerous features and long-term attractiveness of the ESRF, it's vital to attract new member and associate member countries and to enlarge the user community, particularly to include industry and innovation. Part of this effort, he said, requires the laboratory to respond to societal themes – a point exemplified by the energy workshop in which everything from solar cells to new nuclear fuel designs was discussed (see p10).

Director of research Serge Pérez explained how the GIANT partnership of Grenoble science institutes was established to focus on precisely such themes, and that this effort will be boosted by the new €12 m science building scheduled to start construction this year. This joint ILL–ESRF facility funded by the local authorities will host scientific partnerships between research institutes and universities.

To command the changing landscape of European synchrotron science, the ESRF is also strengthening partnerships beyond the Grenoble campus. The ELISA project coordinates a network of 13 000 users, 13 synchrotrons and eight free-electron lasers across Europe, and was recently funded until 2018 under the new name CECILIA. Pérez also listed a raft of acronyms belonging to projects that have been proposed to link individuals at different European institutes, including industry. Agreements with Portugal and South Africa for structural biology and palaeontology research, respectively, are at an advanced stage.

Crucial for tailoring the ESRF beamlines to

particular science themes is a new procedure for beam-time allocation. "Take the example of surfaces and interfaces science," director of research Harald Reichert explained to *ESRFnews*. "Currently the beam-time allocation panel for surfaces and interfaces science deals with applications for beam time on BM32, ID03, ID10, ID15 and a host of other beamlines, but there are 10 other committees sharing the beam time on all of those beamlines, so we could be missing out on efficiencies."

He continued: "Currently, the only way to promote new scientific themes is to set up new committees, but that just fragments things further so we need [to implement] a more streamlined system."

The project received SAC and Council endorsement last year, and is due to start in 2012. In the mean time, a website updating users with the status of beamlines – a need that was highlighted during the structural biology parallel session this year – will be available in the next few weeks or months.

Building on the past

The ESRF's beamline portfolio will be reconsidered in the future, and Francesco Sette has said that he is "personally engaged" to return to a portfolio of 30 public beamlines as soon as practically possible. "Things are changing, but we need to build on all of the beautiful things we have done in the past," he told *ESRFnews*. "You've always got to be a few steps ahead. Had we not initiated the upgrade back in 2003 it simply wouldn't have happened today."

Matthew Chalmers

Energy futures on the agenda

Materials that can help build a sustainable-energy future were the subject of a three-day workshop associated with this year's Users' Meeting, where 120 participants discussed everything from carbon sequestration to fusion. *ESRFnews* talked to workshop organiser **José Baruchel**, head of the ESRF X-ray imaging group, to find out more.

Are you optimistic that humanity will move to alternative energy sources before it's too late?

JB: Presently 80% of energy comes from fossil fuels. This will continue to be the case for some years, yet we are near peak oil now so something else has to come up.

How did the workshop come about?

At the level of Grenoble we already initiated collaboration in 2010 between scientists working on energy materials via the GIANT partnership, which focuses on three main areas: energy, communication and health. The workshop is the next step, and extends the collaboration to the European level.

How can materials science help meet our energy needs?

On the one hand, there is the scope to develop cleaner alternatives such as more efficient solar cells, batteries and fuels for nuclear reactors – all of which were discussed at the workshop. But we can also save fossil fuels by developing lighter and stronger materials, say aluminium-based alloys. One presentation even described imaging techniques being used to model reservoir rock for locking carbon dioxide away.

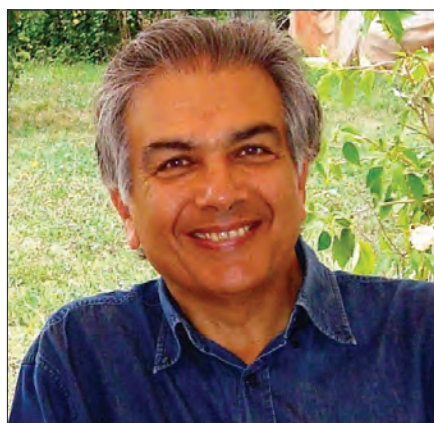
How specifically will the workshop help?

It's a broad community, so we're focusing on materials advances based on neutron and X-ray techniques. The workshop helps a lot because it provides us with the users' advice on how the ESRF and the ILL (Institut Laue Langevin in Grenoble) can even better serve our energy-materials needs.

Is there scope at the ILL and the ESRF for major breakthroughs to be made directly, such as a solar cell with 60% efficiency?

I wouldn't say "solar cells with 60% efficiency", but surely breakthroughs in the future as we understand the mechanisms using neutrons and synchrotron radiation. Some of the technology developed here has been commercialised, such as high-quality mirrors, but usually it's not our job to go up to the industrial product.

That's where GIANT comes in. A lot of the science is produced by our users, and it is through these universities and laboratories that the materials results that are obtained at the ESRF and the ILL mostly can spin out into industry.



"This is not just an academic workshop, but a step towards a natural collaboration with industry."

What was the highlight of the workshop?

I liked hearing about the use of multiple techniques, such as using powder diffraction and imaging to know more about the ion transport in batteries. And it's rewarding to witness the sharing of information in general – we had a lot of different communities together. This is not just an academic workshop, but a step towards a natural collaboration with industry.

What about the impact of your own research?

In light materials we can do real-time 3D imaging of the growth or fracture of a polycrystalline material, knowing in addition the shape and orientation of the grains: this was just a dream a few years ago. These systems can be very close to industrial materials, so I would say that actually opens opportunities and can be considered as a breakthrough.

Were industry representatives present at the workshop?

We had a lot of people from laboratories that are in contact with industry, for instance to study how impurities and defects in silicon correlate with the efficiency of a photovoltaic device, but not yet the guys who actually produce photovoltaic cells.

What is the most important renewable-energy source?

In terms of energy percentage it's currently biofuels, but this can surely evolve.

Will fusion work in your lifetime?

I am afraid "no".

Do we need to orchestrate a sort of "Apollo project" for energy?

The solution is not only technical, but economic. For instance, the French government pushes solar cells by buying the electricity from people who install them and then selling it to consumers at a higher price – essentially a tax to fund solar energy. But the present efficiency of the devices is about 15%, and although we know how to increase that considerably for one-off applications like satellites, the cost is too high for such a system to work generally.

Are there any technical barriers preventing progress in energy-related materials?

Instrumentation has developed dramatically over the last years, but users want to go further all the time. We need more photons, better spatial and temporal resolutions, better detectors, to go faster, and to look over shorter time periods.

Are there more workshops planned?

Yes, and similar workshops are organised in other places, one of them being in Germany in a few months' time. Plus, part of the new science building (here at the ESRF) will host a technology platform devoted to materials for energy, which will bring more cooperation, especially with industry.

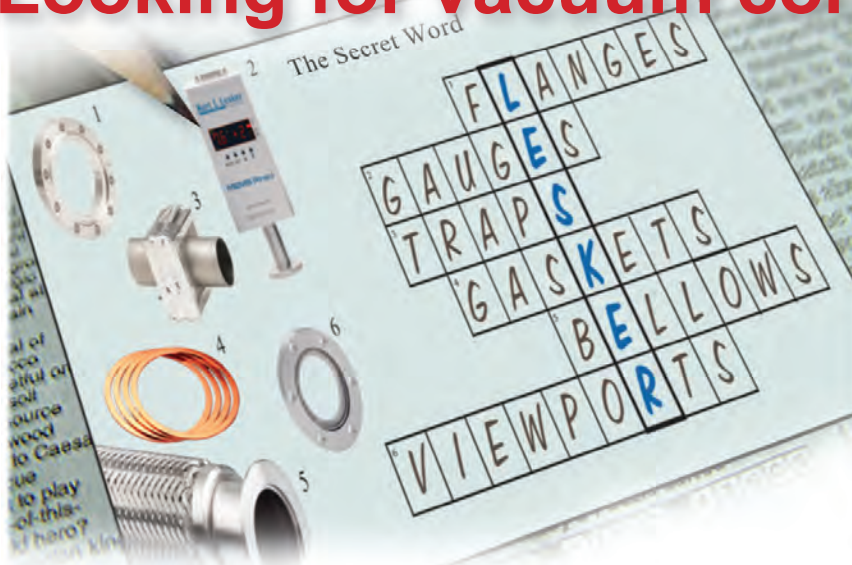
What will be the hot topics in this area 10 years from now?

When I arrived at the ESRF 20 years ago, nobody was talking about having a beamline devoted to microtomography. Today, palaeontology takes up nearly 30% of the time on that beamline, whereas six or seven years ago it was 0%. I can tell you that in five years' time we will still be working on ways to make more efficient use of fossil fuels in parallel with developing alternative energy sources, but I am unable to go beyond that.

Is the societal aspect of your work a source of day-to-day motivation?

When I started out I was motivated by understanding the topic, but at some point I realised that my skills could be used for something with wider impact. Science is much more focused on societal issues now.

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Efficient automation

The ESRF has put in place a future-proofed computing strategy to cover everything from storage infrastructure and data acquisition systems to online data analysis and user interfaces. As *Andy Götz* explains, that strategy is one of the hidden enablers of the laboratory's long-term mission to support data-intensive science.

The fundamental question underlying all computing is "what can be (efficiently) automated?"

The above statement, attributed to the Association of Computing Machinery, is a fitting description of the core computing activity at the ESRF, where efficient automation is very much the headline goal. To understand why, it's necessary to go back to basics. The ESRF is an example of what the late Jim Gray, a pioneering computer scientist, called the "fourth paradigm" in science. What he was referring to is data-intensive science – the other three paradigms being theory, experimentation and computation.

The origin of the fourth paradigm is the so-called "data deluge" resulting from the latest generation of big-science experiments – analytical instruments like the ESRF and the Large Hadron Collider at CERN, among others. The ESRF, for its part, will generate approximately 1 petabyte (1 PB or 10^{15} bytes) of raw data in 2011. What's more, that data output is growing exponentially, creating stresses and strains on the four main building blocks of data-intensive computing: data capture, data curation, data analysis and data visualisation.

So how is the ESRF responding to the challenges posed by the data deluge?

Data capture

Let's start by considering data acquisition. The capture of raw data is still the main source of data at the ESRF; simulation and analysed data are present on a much smaller scale. The challenge for data-acquisition computing is how to handle the very high data rates from the detector to the hard disk. Detectors producing hundreds of megabytes per second are in routine operation today, while the next generation (producing data at gigabytes per second) are already in the works.

Special measures are therefore required to read out the detectors – either using proprietary protocols or multiple Ethernet links – before transferring data to central storage. The key enabler here is high-performance computing solutions for file-storage systems,

and a lot of effort is currently being invested in finding the right combination of network, file servers and buffer computers to handle these high data rates.

Online analysis

Right now, one of the hot topics in ESRF computing is online data analysis. What this means is automated data analysis at the beamline to provide scientists with a first look at the results to get feedback on the quality of the data and to make decisions in real-time about the experiment (see p19).

A key enabling technology in this regard is a framework called EDNA – developed in collaboration with the Diamond Light Source in the UK and other facilities/laboratories – to wrap data analysis programs and automate their execution. The automation can run on a single multicore computer. At the same time, EDNA is being extended to run efficiently on a cluster of multicore computers using a batch scheduler.

For certain applications (such as tomography), it is possible to accelerate online data analysis significantly with the help of graphical processing units (GPUs) – although automating the data analysis depends on capturing the correct metadata during the experiment. Ultimately, the objective is to speed up online data analysis sufficiently to make it attractive for scientists to use. With this in mind, a new user interface based on a workbench concept will enable scientists to set up online data-analysis workflows and browse the results. At the same time, EDNA, which was originally developed for online data analysis for MX, is being extended to other domains like diffraction tomography. In the long term, the goal is to provide online data analysis for all standard techniques and all upgrade beamlines.

Offline analysis

The distinction between online and offline data analysis is very subtle. Online refers to automatically triggered data analysis, whereas offline refers to a manually triggered analysis – though both may run the same data analysis programs. The ESRF has developed



Flick the switch: the ESRF's upgraded data centre will soon be

– and currently maintains – a number of data analysis programs, including PyMCA, PyHST, XOP, Shadow, Fit2D and Fable to mention a few. The ESRF also contributes to programs (like BigDFT) developed outside the ESRF. In fact, the majority of offline data-analysis programs are developed outside the ESRF.

The main challenge for data analysis programs is to be able to profit from the massive parallelisation offered by GPUs and the new generations of multicore CPUs. This involves analysing the existing codes to find bottlenecks and then rewriting to make use of parallelism. Parallelism can bring much bigger performance improvements (speed-ups of up to a factor of 40 have been achieved) versus Grid-based solutions. In 2009, a study was carried out to evaluate the EGEE Grid for data analysis as part of the European Union Framework 7-financed ESRFUP project.

The study concluded that the Grid is unsuitable for data-intensive problems. As a result, the Grid has been abandoned at the ESRF (a change of strategy compared to plans previously outlined in the lab's "Purple Book"). The ESRFUP findings reveal that it is far more efficient to speed up data analysis at the source – using GPUs, for example – than ship huge quantities of data externally and then analyse them. That said, Grid or cloud

and the data deluge



STOCKPHOTO/ARTISTIC

A focus on international scientific collaboration

Innate complexity and human-resource overheads dictate that many instrumentation and software developments in photon science can no longer be undertaken by a single laboratory.

Equally, another significant shift is occurring among scientific users of the ESRF – many of whom now routinely require access to complementary methods (e.g. neutrons and photons) as well as beam time at several synchrotron facilities to complete their investigations.

Such drivers call for much stronger standardisation of practices, data formats, automation, user interfaces and the like. The ESRF is engaged in several large collaborations with partners in Europe and beyond to make progress on these issues. TANGO (<http://www.tango-controls.org/>), PaN-data (<http://www.pan-data.eu/>), LinkSCEEM-2 (<http://www.linksceem.eu/>), EDNA (<http://www.edna-site.org/>) and ISPyB (<http://forge.epn-campus.eu/projects/ispyb>) are well established projects along those lines, while the CRISP and PaN-data ODI proposals will soon be decided upon.

ready to receive its first equipment, including state-of-the-art file servers and tape-based archiving.

computing could still come into play for user communities external to the ESRF working on non-data-intensive problems.

Data storage

The raw product of the ESRF is data. What's more, that data production is doubling roughly every 18 months. Ten years ago, 1 PB storage requirements were difficult to imagine. Today it has become the standard unit for data-producing facilities like the LHC (15 PB/year) and the ESRF (a few PB/year). By way of context, Google processes roughly 24 PB/day. The challenge for the ESRF is to manage these petabyte data requirements efficiently and within budget.

That challenge starts as soon as the data are generated. Issues like which data format, which metadata, how big files should be, which database to use – all these and more need to be addressed. To date, however, these questions have not been tackled in a homogeneous manner for the different experiments at the ESRF.

The MX community has traditionally been the most advanced in managing its data in a database. Over time, such systematic management of data will be extended to all beamlines. This will include the adoption of the HDF5 data format and the generation and

indexing of metadata in a database (to allow the tracking of data and online searching of metadata). These are essential steps towards data curation (i.e. long-term storage to enable data to be reanalysed by scientists other than the principal investigator of the experiment).

Currently, data are deleted after a delay of one to three months after the experiment. This will change as the cost of tape archives drops. Another notable trend is towards open publication of experimental data online (e.g. the PDB database for proteins and the palaeontology microtomographic database).

Inside the data centre

All aspects of computing rely on a properly dimensioned and efficient IT infrastructure. With an eye on the future, the ESRF has invested in a large central data facility that will soon be ready to receive its first equipment. The upgraded data centre will provide a high-quality environment for central data storage, compute power and network electronics, as well as the software needed to access and manage these resources. In terms of specifics, the facility will soon be equipped with state-of-the-art file servers (capable of storing 1.5 PB), a tape-based archiving facility (of several petabytes), compute clusters with a peak performance of 15 Tflops and an

extensive 10 Gbit/s Ethernet infrastructure.

One of the biggest challenges is to provide very-high-performance file storage to be able to write data at high speeds from the beamlines and to be able to read it at high speed during the analysis phase. Such online data analysis places a big strain on file storage because of the simultaneous read-and-write access requirements. The current set-up provides 300 MB/s write access and up to 180 MB/s read access. The goal over the next 18 months is to increase that performance by an order of magnitude without compromising on reliability.

Providing efficient access to compute resources like CPUs and GPUs is essential for online and offline data analysis. For the last 10 years, the ESRF has used the Condor batch scheduler for this task. Recently, a new resource-management scheduler called OAR has been evaluated and the first results are promising. The challenge is to manage resources to better reflect the way that they are used (i.e. as clusters of CPU cores or GPUs).

Against this backdrop of evolving IT requirements, one thing at least is certain: the data deluge shows no sign of slowing. For the ESRF's computing team, the search for ever-more efficient automation goes on.
Andy Götz

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Parallel power: the new rules of reconstruction

Once the preserve of computer-game enthusiasts, graphics processing units have vastly increased the speed of image reconstruction at the ESRF.

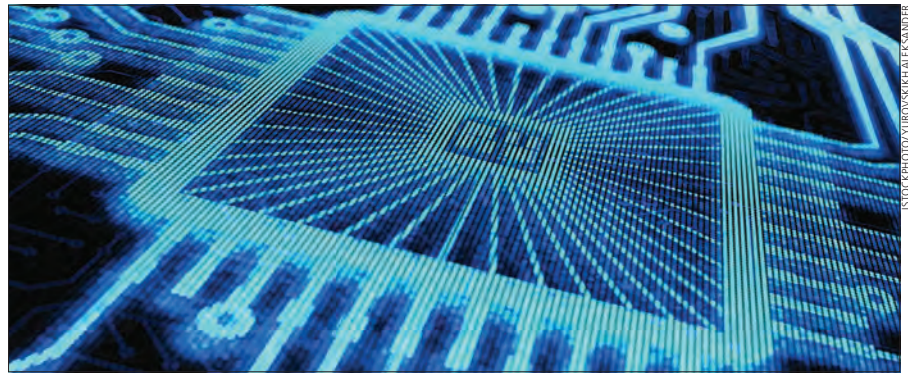
Before last year, everybody at the ESRF knew when the palaeontologists were in town. Processing the huge data sets necessary to reconstruct detailed 3D images of fossils would frequently bring the central computing cluster to a standstill. But thanks to a powerful processor called a graphics processing unit (GPU), the job is now handled by just two computers each equipped with a pair of graphics cards. "GPUs had an immediate effect," says ESRF's Alessandro Mirone. "All the jams occurring on the cluster when huge data sets were reconstructed disappeared."

By integrating GPUs with central processing units (CPUs) to create hybrid architectures, those in the tomography trade are shrinking computing tasks that previously took a day into the duration of a coffee-break. It is now possible to reconstruct data while the scanning process takes place, for instance, and then to use the 3D information to set up high-resolution scans of particular regions.

With the ESRF's beamlines producing raw data at an exponential rate, already exceeding by orders of magnitude the bandpass allowed on the facility's internet backbone, such powerful graphics processing is here to stay. As well as reducing the time during which data need to be stored, the jump in speed allows more compact computing centres and air-conditioning systems, which in turn reduce energy bills. In short, GPUs allow the ESRF to beat some of the limits imposed by its infrastructure. "If one considers a typical 240 W consumption for GPU at full regime and a typical 120 W for a six-core CPU, there can be energy saving for speed-up factors above 12," says Mirone.

Fast fossils

A GPU is a single chip purpose-built to process at least 10 m polygons per second. Originally deployed in the computer-gaming industry a decade ago, GPUs take certain computationally intensive tasks – such as calculating the light reflected off objects – away from central processors, allowing



By integrating GPUs with CPUs to create hybrid architectures, computing tasks that previously took a day can now be completed during a coffee-break.

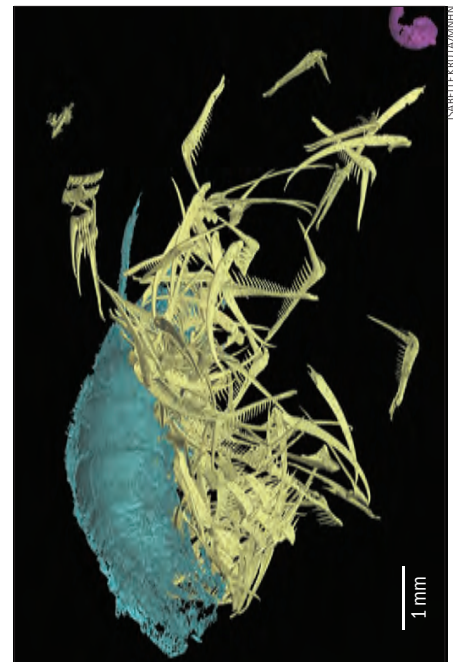
detailed 3D images to be built without slowing the whole system down.

Mirone was a key figure behind the ESRF's GPU revolution. In 2009 he modified ESRF's reconstruction program PyHST (High Speed Tomography in Python), which uses an algorithm to generate a 3D image of an object from a series of projections recorded at different angles, so that the so-called back-projection routine runs on a GPU. It led to a factor of 40 increase in reconstruction speed compared to that using a central processor. "It's the most rapidly gratifying development I ever made," recalls Mirone.

PyHST's efficient use of GPUs helps users to reconstruct 3D images of samples in real time and in great detail, which is very important for studies of dynamical processes and for the multiresolution approaches used in palaeontology. X-ray computed microtomography recently allowed scientists to discern the dining habits of ancient ammonites, for instance, by rendering the jaws and teeth of the prehistoric creature in unprecedented detail, and has been used to study microstructures in the dental enamel of fossil hominids.

"The recent implementation of the Paganin phase retrieval algorithm using GPUs has allowed accelerated processing through a very simple and rapid interface," says ESRF palaeontologist Paul Tafforeau. "Before that implementation, only a few samples could be processed per experiment but it is now used for more than 30% of the ID19 data processing and about 80% for palaeontological studies."

The increased speed of GPUs is also proving invaluable in imaging areas where less data are available and direct reconstruction is not possible. Take the crystal domains and stresses in a material, for instance, which



X-ray synchrotron microtomography is currently the most sensitive technique for nondestructive testing of the internal structures of fossils. This 3D reconstruction, which was generated by palaeontologists working at the ID19 beamline, shows the teeth of fossilised ammonites, distant relatives of squids, octopuses and cuttlefish. The teeth are shown in yellow and the fossil's last meal in blue (crustacean) and pink (snail).

govern how cracks grow in materials and are therefore crucial in the design of more resistant and safe objects. Here, images have to be reconstructed from the limited number of reflected spots activated at certain Bragg angles, which involves solving a set of

algebraic equations. This is a time-intensive iterative procedure, but by porting selected bottlenecks of such algebraic reconstruction techniques to a GPU, ESRF's Dimitris Karkoulis obtained a speed-up factor of 30–40 and the solution now takes a few minutes compared with a day. "Since life cannot be made longer and funding can always become shorter [scarcer], such a speed-up is really precious," says Mirone.

Accelerated simulations

Even before a sample is placed in a beamline, accelerated simulation techniques based on GPUs are proving their worth for ESRF science. That's because they can speed up and increase the reliability of simulations of material properties based on density functional theory, which allows researchers to predict the density of electrons in a system from first principles. Such *ab initio* calculations build images of the electronic wave functions from basic quantum theory, which are vital when comparing theory and observation in great detail.

The program BigDFT, a European project started in 2005, can calculate the electronic structure of ensembles of thousands of atoms corresponding to the size of small biomolecules using massively parallel computer architectures. In 2008 Luigi Genovese of the ESRF Theory Group adapted BigDFT to run on hybrid computing systems

The guts of a graphics processing unit

Graphics processing units, which have been commercially available for just over a decade, operate within a different philosophy to normal, general-purpose processors because they dedicate more silicon to mathematical operation and much less to instructions.

Whereas normal processors need a big amount of cache and a lot of chips for instruction, a GPU has more processing elements. It is made up of tens of multiprocessors, each composed of between 16 and 32 cores, which share the same instructions while working on different data.

in which different sections of the code are ported to run on a GPU. This work, for which he was awarded France's 2009 Bull-Joseph Fourier Prize, has delivered unprecedented performance in the prediction of new material properties – with execution times up to 20 times shorter for some operations. As a result, BigDFT can now tackle systems with larger numbers of electrons (such as metals), taking density functional theory into new realms of prediction.

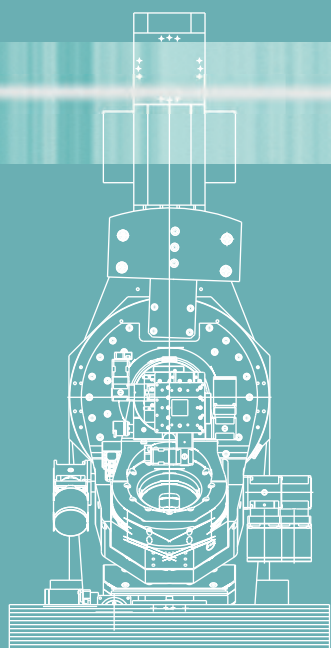
GPUs clearly have a bright future at the ESRF, and one area currently under discussion is their use in modelling the number of rays delivered to an experiment. To ensure that

Provided all of the "threads" – a flow of data and instructions – follow the same path (i.e. they are "non-divergent"), a multiprocessor can be programmed to execute an instruction on all of the cores at the same time. This leads to massive parallelisation – a bit like having several chickens on a single spit and roasting them all with the same rotation.

An algorithm that performs lots of repetitive tasks with independent data, such as adding two matrices, can therefore be accelerated by "porting" it onto a GPU.

users can carry out their experiments, they need to know the effect that the optics has on the rays – something that requires large Monte Carlo simulations. By porting some of the simulated ray-tracing onto GPUs, changes in beam configurations can be calculated faster, thus potentially allowing more rays to be used and better images produced.

"The future processing cluster will be equipped with many GPUs," says Tafforeau. "Then we are expecting incredible increases in processing speed, although the growing size of tomography data sets will continue to push processing to its limit."
Matthew Chalmers



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Materials science: keeping up with the data explosion

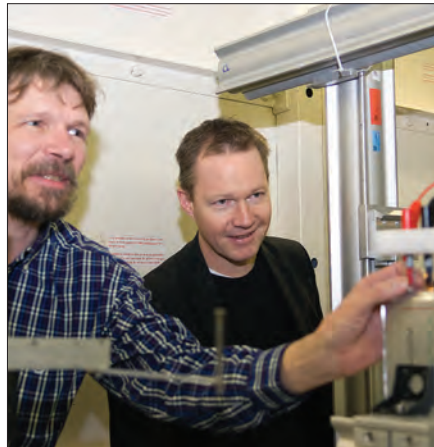
Computers in the ESRF's materials-science beamlines will soon have to deal with terabytes of data per day, all of which will have to be analysed and delivered to users in a matter of minutes.

When the ESRF switched on in the early 1990s, its materials-science beamlines were equipped with just a single workstation. Back then, diffraction data were recorded on image plates that were read out offline. But the arrival of CCD cameras unleashed a data explosion. In terms of image sizes, the first CCD detectors used to produce a couple of megabytes, whereas today's produce up to 24 MB. The new detectors also read the data out much faster: where it once took eight seconds it now takes less than one, and soon will be even quicker. With multiple detectors often in use and frames being recorded every few seconds during an experiment, huge demands are being made of ID11's computing resources.

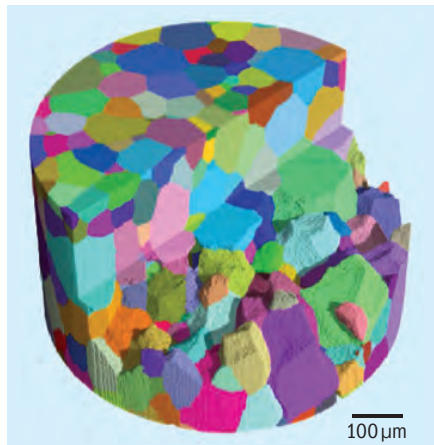
"Since we moved to taking data with 2D detectors, we've struggled to keep up," says Gavin Vaughan, scientist in charge at ID11. "We're taking data faster and faster."

Storing those data is not such a problem. In the past 10 years the ESRF moved from tape storage, which held a few gigabytes, to portable hard drives that can carry a terabyte or so. But thanks to Moore's law, the 40-year-old trend that sees computer-storage capacities double every two years or so, the hardware has kept pace. "Our detector expansion is slower than Moore's law, so things are getting easier for storage," says beamline operation manager Jonathan Wright. "A big helper has been popular demand for large-capacity hard drives for the home PC market, which has made them very cheap." Wright also says that parallel programming will be needed in order for the group to benefit from Moore's law and meet future challenges. "Many existing algorithms might easily be parallelised, but there is still a significant cost to do that. Some GPU codes already exist, but these are not yet in a user-friendly state."

X-ray diffraction methods at ID11 give users access to the structure of materials on a wide



"We are constantly using bigger and more detectors," explains Gavin Vaughan (right), scientist in charge at ID11.



X-ray diffraction contrast tomography reveals the 3D grain shapes in a beta-titanium alloy, a material used in aircraft and engines.

range of length and time-scales. The basic technique is based on analysing diffraction spots produced by grains in the sample, which give scientists the information they need to deduce a material's properties or to study chemical reactions. As is the case at most ESRF beamlines, users need to perform as much online analysis as possible. But the detectors produce a lot of raw data, and algorithms that transform these data into images that users can evaluate require intensive processing. The initial software used in grain mapping experiments, which was tied to a proprietary system that prevented optimisations, used to take months to process a data set. "Now it takes a couple of hours," says Vaughan.

The improvement was thanks to a five-year

EU funding injection, which enabled postdocs at the ESRF and at other institutes to work on algorithm development and implementation until last year. The project, called TotalCryst, was set up to extract the most from ID11's 3D X-ray diffraction microscope, which allows non-destructive characterisation of individual grains and sub-grains inside bulk materials. Practically, TotalCryst provide algorithms that quickly reveal multiscale dynamics of the individual embedded grains. The code has all been translated to modular programs using C or Python, and is now being developed in an on-going project called Fable by staff at ID11 and the Technical University of Denmark.

Bigger, better, faster

Diffraction contrast tomography, a recent and related technique to the 3D microscope, combines microtomography with diffraction to produce terabytes of raw data mapping the 3D grain shape and orientation in polycrystalline materials (see photo, left). All these data have to be corrected and then back-transformed to get from reciprocal space to 3D space to allow users to investigate the growth of grains during annealing and to study the interaction of fatigue cracks with microstructures. It's another area where GPUs are likely to come to the rescue.

"In terms of challenges, there are always new ideas coming up," says Wright. One is the 3D X-ray detector commissioned in 2009 that consists of three semi-transparent screens, which produce a series of three X-ray images at different distances from the sample. This should allow the spatial and angular distribution of the diffraction to be recovered, allowing heavily deformed materials to be studied. The Grain Tracking group at ID19, which is migrating many of its experiments to ID11, is developing a large body of code to derive 3D grain maps on the ESRF computing cluster, but mapping plastically deformed samples is a big challenge. Another challenge, says Wright, is to run analyses in more online modes so that users can get more feedback during experiments; also to maintain software packages developed by postdocs or scientists on short-term contracts once they have left the ESRF.

"We are constantly using bigger and more detectors, and improvements in the beamlines mean data come in faster," explains Gavin Vaughan. "Experiments currently produce about 1 TB per day, but this will be 16 TB in the future and we currently have no way to deal with that!"

Matthew Chalmers

Structural biology pushes the limits of productivity

Automated processing in the ESRF's macromolecular beamlines is fuelling an explosion in activity among structural biologists.

Producing more than a quarter of the ESRF's publications, the scientific output of the macromolecular crystallography (MX) beamlines is unrivalled. The technique, which uses fixed- and tunable-wavelength X-rays to study crystals with unit cells comprising tens of thousands of atoms, is the predominant tool used by a huge community of biologists vying to determine the structure of proteins. "The first structure that I worked on took more than 20 years to solve," says structural biology group head Sean McSweeney. "Now, thanks largely to synchrotrons like the ESRF, the job can be done in a PhD project."

More than 100 000 sample screenings take place each year in the structural biology group's seven beamlines at ID14, ID23 and ID29, leading to 20% of the world's (half of Europe's) solved protein structures, while the pharmaceutical companies that use the MX beamlines for drug design constitute a significant part of the ESRF's industrial activity. It's therefore little surprise that the structural biology group is the second biggest consumer of the ESRF's computing resources after the imaging group.

Automation is key

When it comes to evaluating the large unit cells of biological molecules, crystals are often not of sufficiently high quality for diffraction. MX studies therefore require a lot of computational muscle to evaluate large numbers of screenings quickly so as to allow users to plan their experiments. "Preprocessing requires both good CPU and fast input/output operations to disk, while post analysis requires more CPU and good graphics," says McSweeney.

Once full data are collected, experiments generate large numbers of big images, which must be compressed to allow for easier storage and archiving. While MX shares similar data-reduction requirements as all high-throughput image-based techniques, such as tomography, the structural biology community has common standards on data formats to aid reproducibility and validation. Unlike in tomography, however, the programs currently used by the MX group are unlikely to



ANDREW MONTREUX

"It's mandatory to share a common framework for data analysis," says ESRF's Olof Svensson.

profit much from the faster speeds of graphics processing units.

Preprocessing will become more crucial as biologists tackle ever more ambitious structures, such as complex membrane proteins, in which there is considerable variation in diffraction quality both within and between crystals. Data-collection facilities will also have to be optimised to manage low-resolution diffraction data from very small crystals. The group's priorities this year are to get the system optimised to allow users to sort bad crystals from the few good ones as fast as possible.

Since an automatic sample changer was installed at MX beamlines in 2005, the number of structures elucidated has risen three-fold. To meet the growing demands of structural biologists, further automation will be a major feature of the ESRF upgrade beamline UPBL10, centred around a new sample evaluation and sorting facility called MASSIF. A third of users already operate and monitor their experiment in real time remotely from their home institute via the MXCube interface.

Techniques employed on the other beamlines may vary significantly between users, in contrast to the MX beamlines. But the analysis shares the same basic features: large quantities of data, established algorithms for data reduction, and systems that provide rapid feedback to the user, so other beamlines also stand to capitalise on the high levels of automation developed in the MX area.

The success of the MX automation software developments was partly due to strong collaboration between teams both inside the ESRF and between other European synchrotrons. "We have therefore now started to work jointly in the ISDD software group for implementing automation based on developments done for MX on all of the ESRF beamlines, starting with ID22 and ID21,"

says ESRF's Olof Svensson, who shared the 2008 Bessy Innovation Award on Synchrotron Radiation for his role in developing the customised software used on the MX beamlines.

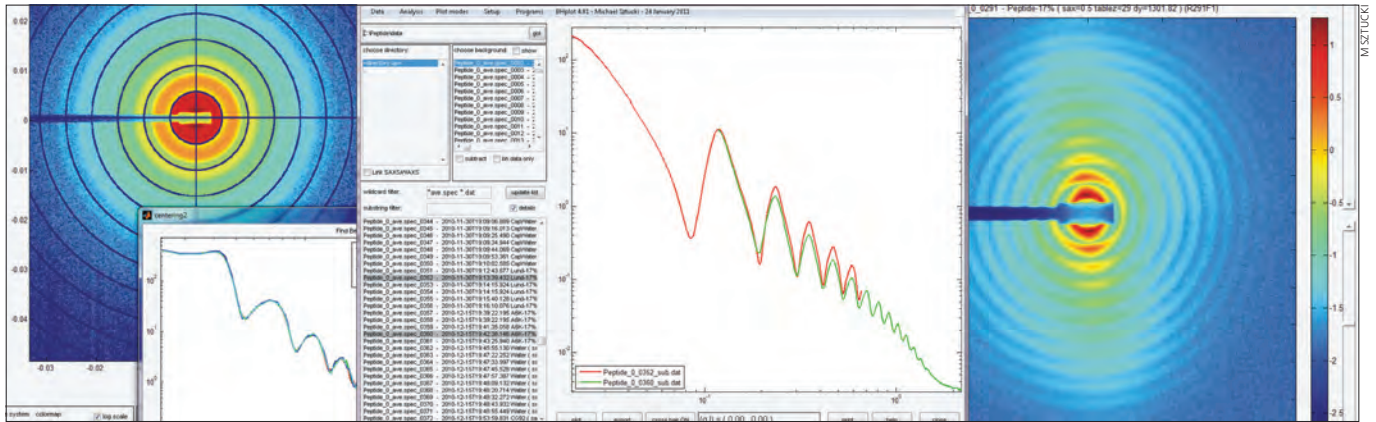
Merging science

Interdisciplinary subjects such as nanoscience are blurring the boundaries between beamlines as different groups employ similar techniques. A biologically oriented SAXS beamline called BioSAXS has recently been installed at ID14-3, for instance, and will allow users to determine low-resolution structures of proteins that cannot yet be crystallised. The framework for automation is the same as that used by structural biologists – and developed by Dimitri Svergun at EMBL Hamburg over the past 10–15 years – while the data-reduction software was inspired by algorithms used on the materials-science beamlines. "It's mandatory to be able to share a common framework for data analysis, otherwise it is much more difficult to make such re-use of software developments," says Svensson.

In summer 2010 a new Dectris Pilatus 6M pixel detector was introduced on the MX beamline ID29, which is capable of running with quasi-continuous read-out. This enables new ways to collect data but puts severe strain on data transfer and processing. Given that this detector could be upgraded to even higher operational speeds, along with the addition of fast detectors on many non-MX beamlines, the ESRF faces the urgent task of providing faster data analysis in general – allowing scientists to leave the ESRF without having to transfer of huge volumes of raw data. To cope with the MX data deluge, the SB's dedicated computing cluster will be significantly enhanced with more processors, faster file access and major database developments.

Matthew Chalmers

SAXS speeds ahead with real-time visualisations



Online data reduction in the ESRF's structure-of-soft-matter group is vital in allowing users to make the most of their beam time. And there's more to come.

You're back at your home institute analysing gigabytes of raw data collected at the ESRF during several days of experiment. You spot something unusual. To properly investigate, you need to change the sample's concentration or view it at a smaller scale. But your beam time is up. You wish you could turn back the clock to have just another few minutes in Grenoble.

Thanks to the online computing resources in the ESRF's structure-of-soft-matter group, users can visualise the results of small-angle scattering (SAXS) measurements in real time. SAXS probes the nanostructure and non-equilibrium dynamics of materials in which thermal fluctuations are sufficient to alter their properties on time-scales of a millisecond or shorter. Examples range from liquid crystals and polymers to granular materials and self-assembling amphiphilic molecules.

Online processing

The SAXS detectors produce hundreds of gigabytes of raw data per day from X-rays scattered at small angles due to nanoscale order in the material. While online preprocessing is a routine part of many experiments at the ESRF, the ID02 beamline is uniquely equipped to reduce data from multiple 2D time-resolved detectors online. The first step is to correct for detector imperfections, such as geometric distortion. Next, the 2D spatial coordinates have to be transformed to polar coordinates and then azimuthally integrated to obtain 1D scattering profiles as a function of scattering vector. Finally, the results must be fitted with functions using a MATLAB-based program,

allowing researchers to derive or infer real-space structure.

With data acquisition times in the millisecond range, a lot of processing power is needed for the online data reduction to match the high frame rate. "We put a lot of effort into the software to enable this," says ID02 scientist Michael Sztucki. Staff in the structure-of-soft-matter group have developed a data analysis package that can operate simultaneously with several detectors and has a graphical interface. The software is written in Python, and the data from different detectors can be processed in parallel.

"You can produce a very large amount of data but their worthiness need to be cross-checked," explains ID02 scientist in charge, Theyencheri Narayanan. "The online processing of data allows us to detect and eliminate many pitfalls in typical scattering experiments at an early stage."

Online processing of raw data is also vital in ID02's anomalous scattering experiments (ASAXS). By recording data at various energies close to the X-ray absorption edge of a certain element, ASAXS experiments can determine the position of that element in the structure. But changes in the intensity due to this anomalous scattering are tiny compared to artefacts arising from the measurements at different energies. Michael Sztucki and co-workers have used ASAXS to deduce the spatial distribution of counterions, providing a crucial input to theoretical models of complex soft-matter systems dominated by electrostatic interactions. And in "kinetic" experiments that investigate the spontaneous self-assembly of soft-matter systems, the

data-reduction software allows researchers to evaluate the robustness of pathways followed in the self-assembly process.

Other beamlines in the ESRF structure-of-soft-matter group will soon have online data-analysis schemes. ID10 is one of them. The goal is to allow intensity-intensity autocorrelation functions of 2D scattering patterns to be calculated online at the rate of 1000 frames per second to derive or quantify the dynamics of the system, which is currently performed offline.

Structural simulation

In ID13, users need to study the orientation of the nanostructure as a function of position, for which 2D patterns are the most useful because the systems are not isotropic. And at ID09, where photosensitive systems are probed by X-rays after a pump laser pulse to see how they change the structure, users rely heavily on molecular dynamics simulations. Here, the challenge is to calculate the time-dependent atom-atom correlation functions, which requires *a priori* knowledge of the system, and users then extract a solution iteratively by simulating tens of thousands of 3D structures. This modelling is especially intensive computationally when, for example, extracting low-resolution structure from non-crystallisable proteins in solution.

"The workstations are all pretty new so we don't need any major hardware at this time," says Sztucki. "One issue for the group is finding the time to develop analysis routines for simulations so that users can extract even more from scattering experiments." *Matthew Chalmers*

Fierce prioritisation is the secret

Itziar Echeverría has taken over as secretary to the ESRF Council. She tells *Matthew Chalmers* how she manages a demanding career while being mum to four young children.

If you hear renaissance songs drifting down from the fifth floor of the ESRF's main building, it could be the voice of Itziar Echeverría, who took up the position of Council secretary and head of the director general's office at the beginning of this year. She has caught herself humming in the past, but her old office was at the end of a corridor so she didn't have to worry too much. "I love to sing," says Itziar. "I have been singing all of my life – outside work, of course."

After seven years as the ESRF's internal auditor, Itziar's new role is to ensure smooth and constructive relations between the Council and the ESRF management, while also providing daily advice and support to the director general. Having met Itziar in her sunny fifth-floor office, I suspect that she would shun the stereotypical "superwoman" title. But as well as managing a top-flight career, she has four children aged seven and under. "I try to set all of my priorities right," she says. "It's complicated, though, and I still haven't got all the answers."

New phase

For someone not especially keen on politics, Itziar finds herself at the heart of negotiations to steer the ESRF through a landscape of budgets cuts, increasing competition and new opportunities. "This is a difficult but also very interesting and dynamic time for the ESRF," she says. "We need to find new sources of funding and safeguard the ESRF's world leadership in synchrotron science, but this can also help us expand to other scientific communities and countries and to be more open to industry."

Itziar hasn't studied science, but it's no surprise that she was attracted to one of Europe's biggest scientific facilities: her father and two sisters-in-law are physicists. "Science is something where I felt I had a foot on already, and the fact that the ESRF



CHANTAL ARGOUË

"This is a difficult but also very interesting and dynamic time for the ESRF."

was also international made it immediately attractive," she says. "That one can carry out a high-pressure experiment at the ESRF and find out about the role that iron and other materials play in the Earth's core, for instance, is wonderful."

Itziar says that her business and legal background is the most important factor in her new job, and points out that a purely scientific background would not, unless it was sufficiently senior, have given her the knowledge of the ESRF gained from her role as internal auditor.

One of the problems that she found when moving from the business to the scientific world in 2003 was that she took it for granted that people at the ESRF understood her purpose. "Before, I was dealing with people in companies who are used to auditors, but at the ESRF I soon

realised that I had to explain myself better and to prepare some of the people to stop them thinking 'my God, the DG is sending me his internal auditor – what have I done?'" The major reward, says Itziar, was when missions came to a close and everyone saw the benefits.

Juggling act

A typical day for Itziar starts at 6.30 a.m. and by nine she's at her desk for a briefing with the DG. "I arrive with my agenda and on-going issues in my head, otherwise I would sink." Meetings often occupy a good part of her day but she tries to keep late afternoons free, when she gets work done at her computer. You won't spot her often at the canteen, but perhaps outside if she takes a lunchtime run. She arrives home after six. "If I don't have something urgent

Echeverría in brief

Born
1974.

Family
Married with four children.

Education
Masters degree in economy and business administration, Universidad Autónoma de Madrid.

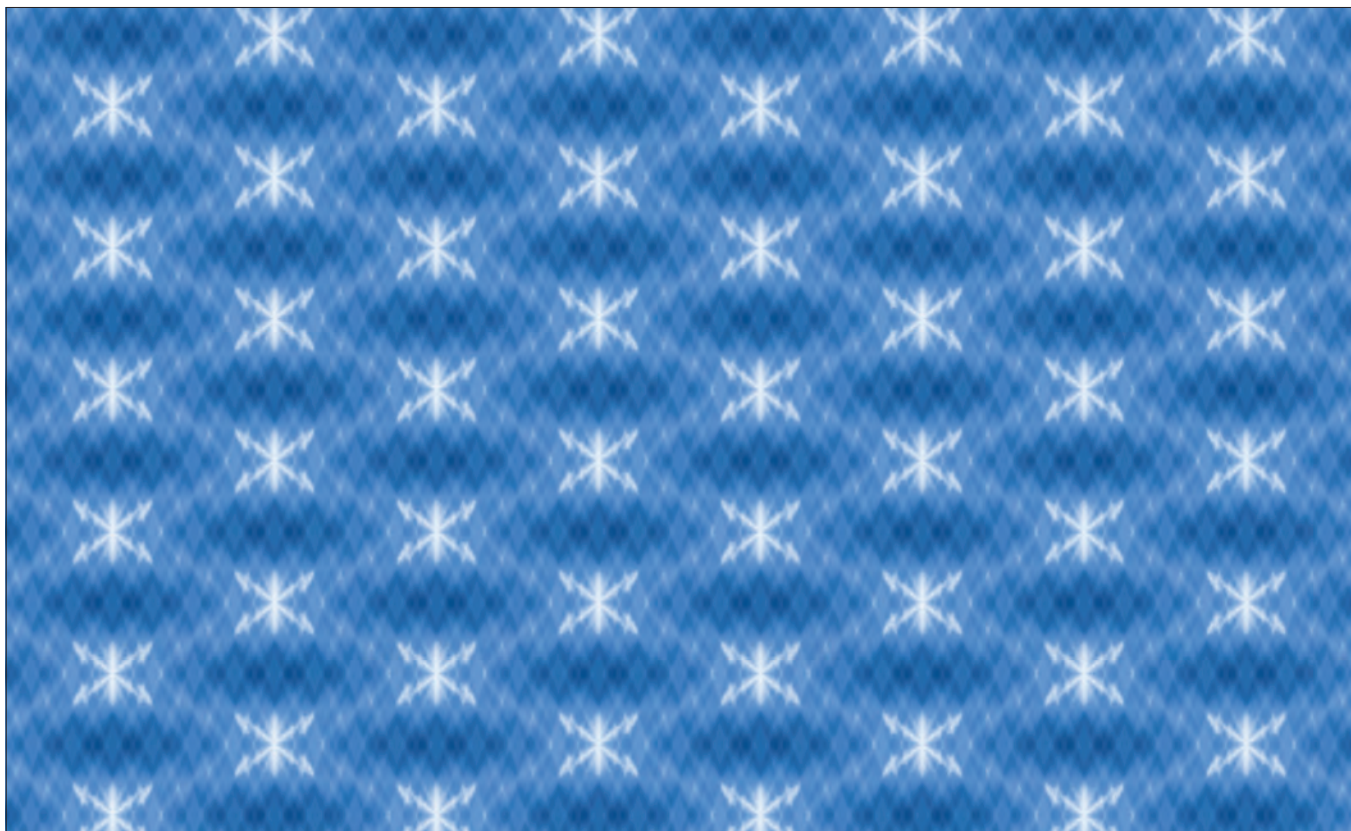
Work
2011: Secretary to ESRF Council
2003–2010: ESRF head of Internal Audit Service
1999–2002: legal and external audit, PricewaterhouseCoopers, Madrid
1998–1999: Ciss Praxis, Madrid

Likes
Singing, running, skiing, cooking and reading.

that requires that I stay late in the office, I'll take care of my children until their bedtime and then sometimes I connect remotely and continue working."

Every so often she finds it hard to sleep, and admits a healthy addiction to tea. As for juggling the demands of a career and parenthood, she says that she benefits from having a husband who supports her 100%. At the same time she reckons that it's all about the quality of the time you spend with children. "It would not be wise taking all four on my own on a day-off like on a Wednesday, so every now and then I'll take one or two of my children and have a really great time at the pool or something."

The previous two secretaries to Council have gone on to be directors of administration at big facilities, but Itziar says that she is not somebody who has a clear career goal in mind. "I prefer to see where the job takes me. If at some point I do have to sacrifice something, it won't be my family."
Matthew Chalmers



RENEZANETTE

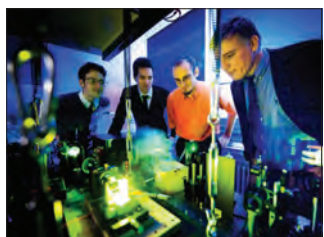
Talbot carpet: They resemble snowflakes, but in fact are simulations of what happens to a plane wave that has passed through a phase-shifting line grating. Self-images are observed at different planes along the optical axis (horizontal), a phenomenon first observed by the photographer HF Talbot in 1836. Today, the Talbot effect is used to produce high-sensitivity phase-contrast and scattering-contrast X-ray images of biological and palaeontological specimens. An advanced 2D grating interferometer has recently been demonstrated at ESRF (*Phys. Rev. Lett.* **105** 248102).

In the corridors

Collapsed light offers exotic source

Against all the odds, researchers have created a new light source by coaxing photons into a macroscopic quantum state called a Bose-Einstein condensate. BECs were first created in 1995 from rubidium-87 atoms, which have integer spin (bosons) and can therefore collapse into the same ground state when cooled to extremely low temperatures.

But photons, the most common boson, were thought to be immune from such a phase transition because they are too easily absorbed by surrounding



Coaxing photons in novel ways.

UNIVERSITY OF BIRMINGHAM

apparatus. The team got round this by allowing the photons to thermalise with a dye in an optical microcavity. The result could lead to novel light sources that resemble X-ray lasers, with applications in photovoltaics and semiconductor chip manufacture (*Nature* **468** 546).

Data deluge quantified

It makes the ESRF's annual data output of one petabyte (1 million GB) look minuscule. Researchers at the University of Southern California have calculated that humanity has amassed 290 exabytes of data (290 billion GB), having surveyed 60 different media from books and X-ray films to hard drives and credit card chips in the period 1986–2007 (*Science* DOI:10.1126/science.1200970).

The survey showed that the "digital age", when digital overtook analogue storage, began in 2002. Before 2000,

three quarters of stored information was in an analogue format, but by 2007 94% of stored information was kept digitally. Global computing capacity also increased by 58% per year during the two-decade period.

While 290 exabytes is indeed large, it is smaller than the 1.9 zettabytes of information transmitted in 2007 through broadcast technology, such as TVs and mobile communications. That's possibly equivalent to everyone in the world reading more than 1000 copies of *ESRFnews* per day!

Got a bad project?

A biology-themed parody of Lady Gaga's hit song *Bad Romance* has racked up over 2.3 million hits on YouTube. Performed by researchers into Alzheimer's disease at Baylor College of Medicine in Texas, the song – titled *Bad Project* – includes memorable lines such as: "I want



Oh oh oh... caught in a bad project

Going Ga Ga with a project from hell?

good data, a paper in *Cell*, but I got a project straight from hell." It's a must-watch for graduate students of all disciplines.

X-ray meeting

Resonant Elastic X-ray Scattering 2011 (REXS 2011), bringing together researchers from different fields in condensed matter who use elastic small- and/or wide-angle scattering techniques, will take place in Aussois, France, on 13–17 June. Places are limited to 150, and registration closes on 1 May. More information is available at <http://rexs2011.grenoble.cnrs.fr/>.

YOUTUBE

EX2 is all about planning and execution

Building engineer Paul Mackrill explains why EX2 is no average construction project.

Nanoscale beams are a key feature of the ESRF Upgrade Programme, opening a new era in imaging and measurement at the smallest scales. But focusing beams to such extremes requires beamlines up to 250 m long, entailing new buildings on 21 000 m² of raw surface area.

At least, that was the original plan. The shortfall in the ESRF's budget has meant that the Vercors extension on the south side of the storage ring has been cancelled, and the smaller Peninsula extension on the north side has been replaced by a satellite building. The present project, involving two extensions called Belledonne and Chartreuse on either side of the main building, requires 12 700 m² of raw surface area.

That doesn't make the task of building engineer Paul Mackrill, who along with project manager Emmanuel Bruas is responsible for the experimental hall extension project (EX2), much easier, however. "It simplifies some of the planning because the impacted areas involved moving lots of people, and obviously we make a big saving by not building the buildings," says Mackrill. "But we still had to do the planning and design because the buildings



The main challenge facing the EX2 team is planning to ensure continued use of the existing facility with minimal disruption to users.

shared much in common."

It's not just a case of making buildings bigger, either. Increasing the capacity of a beamline also requires extra services, one being a ventilation system that keeps temperature changes to within ± 0.5 °C to ensure that experiments are unaffected. A well insulated building is crucial, and this will be helped by covering the roofs of the new buildings with grass turf. The primary function of the turf, however, is to reduce the run-off from rainwater.

The huge concrete slab that forms the building floor also needs the temperature to be as stable as possible to avoid deformation. This 4000-tonne, 1 m-thick monolith is the centrepiece of the upgrade's beamlines, and it occupies a big chunk of Mackrill's time. "I

call it the golden slab to make people – in particular the external engineering company – realise that it's different from previous slabs," he explains.

The first 70 cm will be a low-strength concrete called Rollcrete that has been compacted rather than poured by a machine, followed by a layer of bitumen and finally a 30 cm thick reinforced slab on top. Having a single slab – 2400 m² for Belledonne and 1600 m² for Chartreuse – is vital for stability and to allow the layout of the beamlines to be changed as required. The top layer alone should take three days of carefully and continuously pouring concrete from the centre outwards.

The final design has not yet been signed off, but after three years of work the team is

currently carrying out the detailed specification ahead of the call for tender, which goes out in April. The site will be prepared in September and major ground broken in December, with construction rolling on to May 2013. "We've timed the major construction to fit between December 2011 and April 2012, but it's very tight," says Mackrill.

The main challenge now facing the EX2 team is planning to ensure continued use of the existing facility with minimal disruption to staff and users. "You can't just do what you want to," says Mackrill. "Once we've got the technical issues solved, such as making sure the concrete provider can deliver the high specifications that we require, we have to closely check the phasing of all the activities."

EX2 is not your average construction project, and the team has also worked hard to be as energy-efficient as possible. As well as keeping the buildings' energy bills as low as possible, the debris during construction will be sorted and any waste minimised. "There already exist national regulations for this, but we're going even further," says Mackrill.

Matthew Chalmers

Movers and shakers

Innovation award



ESRF scientists Anatoly Snigirev and Irina Snigireva (left) have been

awarded the 2010 Innovation Award on Synchrotron Radiation for the joint development of compound refractive X-ray optics. Simple to align and easy to operate, refractive X-ray lenses are used in half of the ESRF beamlines and at numerous other synchrotron facilities worldwide. It is the third time that ESRF staff have won the Society of Friends of Helmholtz-Zentrum Berlin prize since its inception in 2001. The Snigirevs share the prize with former ESRF director of Research

Bruno Lengeler (now professor emeritus of RWTH Aachen) and Victor Kohn of the Russian Research Center Kurchatov Institute, Moscow.

New users' head

At the Users' Meeting dinner on 8 February, Gerlind Sulzenbacher handed over her responsibilities as chairperson of the Users' Organisation to fellow Italian Chiara Maurizio from the University of Padova and formerly at the Italian CRG beamline at the ESRF. Replacing Gerlind as structural biology representative is Beatrice Vallone of the University of Rome "La Sapienza", while Chrystèle Sanloup of the Institut

de Physique du Globe de Paris replaces Tullio Scopigno as the representative for dynamics and extreme conditions.

Council chairs change

Former vice-chairman of the ESRF Council, physicist Jean Moulin, has taken over from Robert Feidenhans'l as the new council chairman. Director general of the SOLEIL synchrotron, biochemist Michel Van Der Rest, has been appointed vice-chairman of council.

Congratulations

• ESRF's Wilson Crichton from the Dynamics and Extreme Conditions group has become a member of the Mineralogical

Society of America.

• Former ESRF director of research (2003–2009), Sine Larsen, has taken over as interim director of Sweden's MAX IV laboratory as of 15 February.

Röntgen prize for ESRF users

Christian David of the Paul Scherrer Institut and Franz Pfeiffer of TU Munich received the Röntgen prize for their joint development of grating-based phase contrast with conventional X-ray tubes, work that was originally based on experiments carried out at BM5 and ID19. The pair recently used the technique, which enhances the quality of X-ray images, to gain new insight into the human brain.

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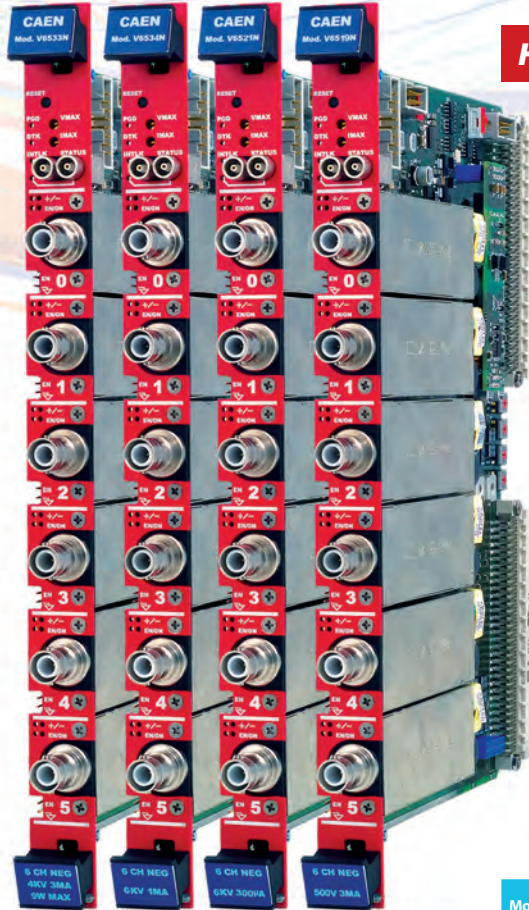
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V6534 P/N/M	6 kV (0.1 V)	1 mA	20 nA (2 nA zoom) ⁽³⁾	500 V/s	10 mVpp (25 mVpp)

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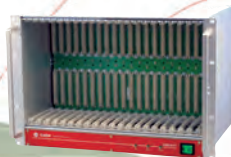


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