Appendix
LEAPS STRATEGY 2030

Strengthening Europe’s leading role in science and innovation

LEAPS League of European Accelerator-based Photon Sources

League of European Accelerator-based Photon Sources (LEAPS)

LEAPS is a collaboration bringing together photon sources each of which produce exceptionally intense beams of X-rays, ultraviolet, and infrared light. These photon sources enable insights, which are not possible with more conventional equipment in both basic and applied research, covering virtually all fields of science from physics, chemistry, and biology, to energy, medicine, cultural heritage, and engineering. They can be considered as 'super microscopes,' which enable research on samples in the tiniest detail, helping make invisible information strikingly visible.

Light source facilities have been working alongside each other in Europe successfully for years, supporting world-class science. In the past five years alone, LEAPS members have welcomed over 24 000 researchers to their facilities, users, who have had an impact on a wider network of greater than 35 000 researchers, culminating in more than 23 400 unique articles published in peer-reviewed journals.

The future holds great promise too: new technologies to produce and exploit yet more powerful light sources have been conceived, with the potential to transform the impact on increasingly complex scientific and societal problems. Realising this promise amid rising international competition requires facilities across Europe to draw even more effectively on their collective strengths, and to do so swiftly.

The LEAPS collaboration offers a step change in European cooperation, bringing together 16 organisations representing 19 research infrastructures (RI) through a common vision of enabling scientific excellence solving global challenges, and boosting European competitiveness and integration. This will be achieved through a common sustainable strategy developed in consultation with all stakeholders, including national policy makers, user communities and the European Commission.

The LEAPS members will produce a road map for the development of the next-generation light sources and instrument technologies, advocate for its funding and together address the big data challenge.

LEAPS will also:

- Play to the strengths of individual facilities through smart specialisation, recognising strengths in a more coordinated way to better serve the future needs of the user community
- Strengthen and expand services to industry in order to trigger innovation more widely and effectively
- Standardise and improve access modes for users, capture and map socio-economic impact, enhance training and outreach programmes
- Strengthen scientific integration, both across Europe and worldwide

Second edition, June 2018

› **5 Nobel Prizes directly linked to our research infrastructures**

› **Over 23 400 unique articles published in peer reviewed journals in the last 5 years from diverse fields of science, making Europe a world leader in research**

› **More than 24 000 direct users and a wider network of over 35 000 researchers**

Vision

A world where European science is a catalyst for solving global challenges, a key driver for competitiveness, a compelling force for closer integration, and an initiative for peace through tighter scientific collaboration.

Mission

LEAPS will use the power of its combined resources to ensure that member light source facilities continue to be world - leading, to act as a powerful tool for the development and integration of skills with a view to address 21st century global challenges, and to consolidate Europe's leadership in the field.

Working together to form LEAPS

Introduction to LEAPS research infrastructures

Modern societies are facing a number of grand challenges in order to evolve into sustainable economies. Solving many of the grand challenges require breakthroughs in materials, processing, and fundamental understanding of nature. These breakthroughs can only be delivered by scientists and engineers using the most advanced tools and full collaboration on an international scale.

The continuous feedback between facilities and of users is an indispensable contribution for the development of facilities and for the long-term sustainability of the transnational access (TNA) support for the users at European synchrotron and FEL radiation facilities. Because European users are presented by an own user organisation, ESUO can provide various kinds of expertise for the development and improvement of future experiment and for expanding to new fields. It fosters exchange of knowledge between various user groups and with users from industry and contributes to the education of the future user communities in the use of synchrotron and FEL radiation.

To date there have been 21 Nobel Prizes awarded in the X-ray sciences, a far higher number than in any other scientific field, reflecting the enormous impact of this community on science and society. The 1997 Prize in Chemistry was the first to be given for work carried out at synchrotrons; all four subsequent Prizes for work using X-rays were also dependent on data from synchrotrons.

Today Europe is home to 13 synchrotrons and 6 FELs located in ten Member and Associate states. Optimal exploitaition of this multi-billion € investment requires collaboration and smart specialisation. The facilities' different energy ranges (0.012 - 17.5 GeV) and specialised beamlines of national communities, provides some intrinsic specialisation; however to achieve a step change in smart specialisation requires trans-European coordination. This is urgently needed to maintain European competitiveness in the face of upgrades and newly built accelerator-based light sources in the US, China, and Japan.

European-wide coordination and smart specialisation as offered by LEAPS will allow scientists from any country and science field to go to the LEAPS facility which is most appropriate for their field of science. This means facilities can specialise in certain experiment types enabled by their technical parameters, or as required for their local community, knowing that other experiments are covered by one of the other LEAPS partners. In addition, standardisation (for example in sample holders, data format, safety and access rules) makes it much easier to move between facilities, thus evading high oversubscription and long waiting times.

Science at Synchrotrons

Introduction

One of the most advanced tools are synchrotrons i.e sources of X-rays produced by ring-shaped particle accelerators. X-rays are photons of high energy that are the ideal tool for investigating the properties of matter due to their penetrating powers, wavelengths that are comparable to interatomic distances, and energies that allow direct investigation of chemical bonds. Over the past decades, synchrotrons have provided ever-higher-quality X-ray beams, allowing scientists to tackle increasingly demanding and societally relevant questions in a multitude of scientific areas.

Because synchrotrons are large and expensive centralised facilities, they foster collaborations between scientists across national boundaries and scientific disciplines. They typically allow many tens of independent experiments to be conducted simultaneously, thus serving a large and diverse community. Today the more than 24.000 European users of synchrotrons represented by the European Synchrotron and Free Electron Laser User Organisation (ESUO) embody an open and extremely innovative community, which is still growing mainly due to the increasing number of users from Eastern Europe countries.

Social and Economic Drivers

Society urgently demands new technologies to deal with grand challenges such as health, energy, environment, food, production, and preservation of heritage. Synchrotrons can contribute to solving these challenges because they elucidate structure and chemistry down to the atomic level in realistic samples and because they naturally bring together experts from all areas of the natural sciences, providing complementary know-how to tackle the most difficult and pressing problems.

Important examples include the development of sustainable materials and processes, for example:

- 85-90 per cent of the chemical products currently manufactured in industry rely on the use of catalysts in one or more stages of their process. Making processes more sustainable, e.g., by using less energy, or creating less by-products and CO_2 (85 million barrels of crude oil are processed per day) will have a huge impact on the environment and the economy. The new catalysts required to support this aim require detailed characterisation at the atomic level and synhcrotron sources are the ideal tool to resolve this information.
- Energy materials, used for storing, transporting and exploiting electric power or chemicals, are increasingly important to enable the use of alternative and clean energy sources, requiring in turn detailed insights down to the atomic level.
- To provide a global clean environment and supply of water, it is essential to be able to measure and understand the impact of pollutants and develop possible cleaning and remedial measures.

- Health, i.e. curing diseases, requires detailed knowledge of biomolecules as well as the actual bio-processes down to a sub-cellular level.
- Preserving our cultural heritage for future generations depends upon gaining an understanding of the object's origin and the ageing and deterioration processes taking place, down to the atomic level, via non-destructive techniques.

Because synchrotron radiation (SR) provides the necessary techniques to analyze a broad range of samples in a non-destructive manner, at relevant conditions, the results have a major impact, advancing both the understanding of existing materials and processes, and the development of new ones. In the next decades, these synchrotron generated discoveries will open up even more exciting business opportunities, enhancing Europe's economic competitiveness.

Science and Technology Drivers

Over the past four decades inventions in accelerator design have increased the brightness (quality) of photon beams by many orders of magnitude.

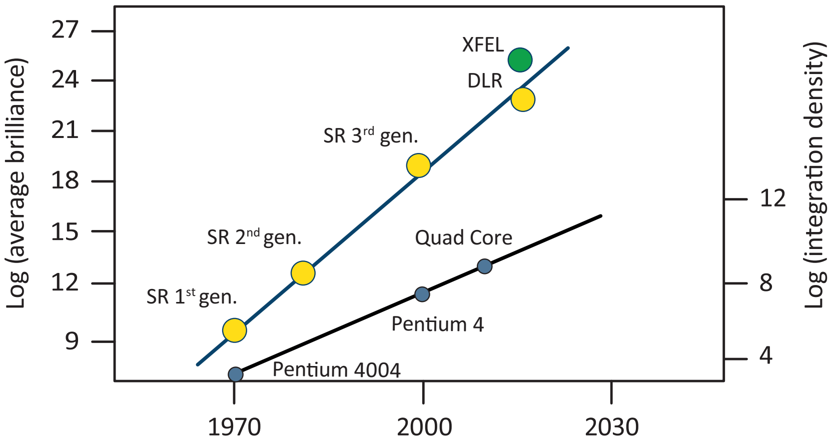


Fig. 1. Comparison of the brilliance of X-rays delivered by photon facilities over the years (LEAPS' law) with the gain in transistor density in integrated circuits (Moore´s law). (DLR = Diffraction Limited Rings with ultimate performance; XFEL = X-ray free-electron laser)

The recent innovation of so called multi-bend achromats has added another factor of 30 or more. Europe is a leader in this field with one facility operating already (MAX IV), another facility in the process of an upgrade (ESRF) and serious planning underway at five more of the 13 European synchrotrons. Competing facilities are being built in Brazil (SIRIUS), while two sources are planned in the US (APS-U, ALS-U), two in China (HALS, HEPS), as well as three in Japan (SPring8-II, Slit-J, KEK-LS).

High-brightness sources deliver more of the photons needed for a state-of-the-art experiment onto the sample. Moreover, high-brightness synchrotrons provide coherent photons, which is a qualitative gain.

This gain in quantity and quality can be used in many ways to enable new science:

- Faster experiments (time resolution), more accurate experiments (higher spectral or spatial resolution), more samples (measuring tens of thousands of samples), smaller samples (sub-micron crystals, precious materials, ...), etc. Experiments, which seem heroic today and require years of preparation and data analysis, will become feasible and available to inexperienced users. This makes the unique benefits of synchrotrons accessible to more scientists and entirely new scientific and industrial communities.
- Higher-brightness X-ray beams also allow progression from the investigation of static structures to transient experiments. It becomes possible to investigate materials undergoing changes in structure or composition, as for example, in fabrication of novel materials, chemical reactions mediated by a catalyst, melting or solidification, or biochemical reactions relevant for human health.

Two specific techniques are emerging that use coherent X-ray beams. The first is coherent imaging, allowing researchers to image samples at circa 10-nm spatial resolution in 3D. The second is X-ray photon correlation spectroscopy, providing information about dynamics and changes in a material with temporal and spatial scales relevant for fabrication and processing of novel materials.

Both techniques are also applicable at FELs, where they will be extended to even higher spatial and temporal resolution for certain samples. The coming upgrades of European facilities will also drive the optimisation of all aspects in the value chain of scientific discovery, starting at the photon source and ending with data analysis.

A parallel development strengthening science at synchrotrons is the disruptive change of 'big data'. Our ability to acquire very large (>100 TB) data sets in multiple dimensions (6 dimensions = 3 spatial + temporal + spectral + load/temperature/composition) and deducing relevant quantitative information is changing the field. Here, machine learning will make complex synchrotron experiments meaningful providing rapid quantitative feedback and solutions to both existing and new users communities.

Science at Free Electron Lasers

Introduction

Free Electron Lasers (FELs) represent a unique class of photon sources that provides radiation over the entire frequency range from mm to hard X-rays which is the foundation for ground-breaking discoveries with FELs in all arenas of natural sciences. They are outstanding tools for investigating matter under extreme conditions and they deliver unique contributions to important problems of societal relevance such as health, energy, smart materials and environment.

FELs are unprecedented bright sources, about 100 million to a billion times brighter than e.g. synchrotrons in the X-ray regime, providing extremely short pulses, down to a few femtoseconds, a combination of attributes which allows researchers to follow molecular motion and perform spatially coherent experiments. These qualities make FELs unrivalled tools that provide the platform to address some of the most challenging and urgent questions of science, technology and society.

The scientific impact of the latest advent of the FEL family, the X-ray FELs, is increasing very rapidly. One of many scientific areas opened by X-ray FELs is the opportunity to study matter which has so far been inaccessible to high-resolution structural examination. A prominent goal is the study of inherently non-crystalline biological materials, such as cells or biomolecules. Furthermore, first experiments in time-resolved structural studies have already been performed with the goal of "filming" a chemical reaction, not just observing the final product as achievable using current analytical methods.

Social and Economic Drivers

Solutions of many important challenges facing humanity, such as developing alternative sources of energy, improving health, mitigating environmental and climate problems and developing new "green" economies, depend on an ultimate understanding and control of matter. While scientific developments in the twentieth century focused attention on understanding matter on the natural length scales of the basic building blocks of matter, the challenge of the twenty-first century is to master the understanding of the dynamics that ultimately governs the function of materials.

Prominent examples include

- The prevention and cure of diseases that requires the complete understanding down to the molecular level and the design of new pharmaceutical products that relies on deciphering the atomic details of the structure of biomolecules. Due to their unique properties, FELs will enable a huge leap in the ability to investigate, visualize, and understand the molecular basis of biological processes. Research in these areas at FELs will support the long-standing fight for the health of an ageing population.

- Solar energy may provide the solution to the various challenges our society is facing in providing the necessary energy to support the industrial output and ensure the comfort and transportation requirements of our daily life. However, direct use of solar energy for generating electrical power or heat is confronted with the need to store energy, as the production cycle does not match the consumption cycle. One possible solution is to make indirect use of solar energy, for instance by artificial photosynthesis. FELs can take time-resolved pictures of such reactions, leading to a much better fundamental understanding.
- Catalysts in chemical reactions are complex, indispensable ingredients which allow efficient progress of reactions. Today, catalysts are widely used, e.g. to limit the environmental damage of car exhaust gases and are fundamental in the petrochemical industry and in many other applications, with a market of tens of billions of euro. Despite their widespread use, the action of catalysts is very often poorly understood prohibiting their rational design. FELs will give new opportunities for understanding the underlying molecular mechanisms in detail and will improve the development of better and more environment-friendly catalysts, with important effects on a whole range of important industrial processes.

Science and Technology Drivers

Free Electron Lasers are excellent examples of large-scale research infrastructure with high scientific and innovative impact. They enable matter, molecules and materials to be taken to the extremes of modern- day technology and define an arena for new discoveries, and by providing state-of-the-art tools they allow researchers to probe, control and manipulate essentially all states of matter, in the solid, liquid and gaseous phases.

Hard X-ray FELs with their intrinsic lateral coherence and intrinsic longitudinal coherence obtained with transform limited seeded FEL beams, are envisioned to be especially powerful in the study of disordered solids and liquids through the use of techniques such as Coherent X-ray Imaging, X-ray Photon Correlation Spectroscopy and X-ray Cross Correlation Analysis. Hard X-ray FELs will enable diffraction studies that elucidate the symmetries of liquids and disordered materials at the interfaces that control reactivity and stability.

Fascinating new scientific opportunities are provided by soft X-ray FELs, for instance by allowing the exploration of the chemistry of carbon, nitrogen and oxygen that underlies some of the most important processes in our world. Life in its present form would not exist without photosynthesis involving the sunlight initiated catalytic conversion of water and CO_2 into oxygen and hydrocarbons. Soft X-ray FELs also allow users to study 3d transition metals which are key to many catalytic reactivity centres exploited in chemistry and the life sciences. The properties of the elementary 3d metals and their oxides are the dominant topic of modern condensed matter physics and materials science.

For example, the elementary ferromagnets Fe, Co and Ni form the basis for information storage in the form of nanoscale magnetic bits, while novel and fascinating phenomena associated with transition metal oxides such as high temperature superconductivity and colossal magnetoresistance not only challenge the existing concepts of condensed matter physics, but these materials may become the basis for a post-silicon technology era.

Intense radiation from FELs in the infrared and terahertz (THz) range of the electromagnetic spectrum acts as a orthogonal spectrometric tool that probes important excitations like vibrations, electronic and magnetic transitions in matter close to their ground state, the natural habit of the system. The region of the electromagnetic spectrum - ranging from the fingerprint regime in the mid-infrared, over far-infrared between the electronics and photonics domains to the THz regime - is uniquely suited for studying and controlling systems such as molecules, clusters and complexes, but also electrons in metals and semiconductors, as well as the collective modes of biologically important proteins.

Future Developments and Capacity

A common trend in research that agenda-setting projects involve large-scale research infrastructures offering unique experimental capabilities as pivotal platforms to push back the boundaries of exploration and help address the many challenges confronting society. In order to understand and eventually control the function of materials in the widest sense, researchers require access to a wide range of wavelengths, methodologies and instrumentation.

The field is rapidly developing and many of the experiments performed with FELs up to now are proofs-of-principle. Future developments of FEL sources will address the possibility to "lase" in a controlled manner by using innovative seeding schemes, to enable the production of two-colour pulses with different time delays, to provide ultrashort pulses, to improve electron and photon diagnostics, X-ray optics, optical lasers and their synchronisation as well as the experimental methodology and instrumentation. Many of these demanding developments are at the cutting edge of current technology providing fertile soil for innovation.

Another challenge is related to the user access capabilities of the FEL sources; these have been implemented initially as facilities delivering beam to one user at a time, meaning operational facilities are only able to accept a fraction of the large user communities interested in their use. The possibility of increasing the experiment opportunities at FELs is still a strategic challenge both for the existing facilities and the upcoming projects, even if with the recent start of operation of two new X-ray FEL sources European XFEL and SwissFEL, both with plans for performing more experiments in parallel, a new era is entered where significantly more user time will be given for FEL scientific and innovation applications.

Thus, a set of complementary FEL light sources, outfitted with a number of complementary beam lines and a variety of experimental stations, will be available to the European scientific community and shall be used in a most efficient way to exploit the enormous potential these facilities offer to a growing multi-disciplinary user community.

LEAPS facilities contribution to grand challenges

Solutions of many important challenges facing humanity depend on an ultimate understanding and control of matter. Synchrotrons and FELs can contribute to solving grand challenges because they have the capabilities to elucidate realistic information down to the atomic level and at relevant time-scales, providing complementary know-how to tackle the most difficult and relevant problems.

Health

The grand challenges – drug resistance and age-related illnesses

The scientific answers – mechanistic understanding, new drugs and personalised medicine

The LEAPS role – leveraging advances in brightness, automation and computation to drive biomedical discovery

The LEAPS impact – standardised databases allowing Europe-wide integration of massive volumes of atomic to tissue level information for machine learning. Efficient and rapid screening of combinatorial drugs.

Scientific research into the molecular mechanisms responsible for the development and maintenance of the human body, and, conversely, for its dysfunction in disease, has underpinned numerous medical advances over the last century. There has been an immense positive impact on the health and well-being of the humankind as a result of the development of vaccines and antibiotics to combat infection, as well as of small-molecule drugs and biologics to treat conditions ranging from rheumatoid arthritis to heart diseases. Over the coming decades, society will face the major threat of currently treatable pathogens developing drug resistance.

Likewise, the shift in demographics of ageing populations poses the substantial challenges of ever increasing healthcare costs and the impact of age-related illnesses such as dementia.

New therapeutic agents will be required to meet the challenges of maintaining a healthy population in the 21st century and to avert the rise of ‘super bugs’. The opportunities for personalised medicine, offering prevention and treatment of disease tailored to the genetic landscape of the individual, offer huge possibilities. However, it also escalates the urgent need for mechanistic understanding and specific drugs, as well raising the spectre of inflating healthcare costs. The next generation of LEAPS beamlines will provide the data-acquisition tools required to accelerate the discovery of novel therapeutic approaches and the design of new drugs and biologics.

The technical advances in synchrotron and FEL beamlines provided by the engineering and physical sciences are directly driving life-science discovery. Current synchrotron beamlines have enabled macromolecular crystallography to provide the atomic-level details of thousands of complex biological molecules and assemblies to inform biomedical research (e.g. data collection at European synchrotrons resulted in deposition of 4,846 coordinate sets into the Protein Data Bank during 2017, 44.6 % of the global total). The development of high-brightness synchrotrons delivering major improvements in the quantity and quality of photon beams, coupled with advances in detectors (e.g. the high-speed Dectris EIGER detector routinely operating at up to 750 Hz), automation (in hardware and software), and computation to tackle huge volumes of data, will offer a sea change in what can be achieved. Automated fragment-screening beamlines will be capable of delivering thousands of structures of target proteins in complex with chemical compounds per day.

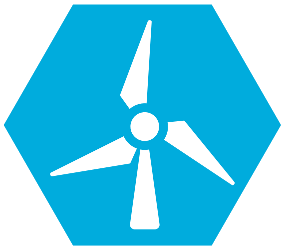
This explosion in the volume of data will fuel a revolution in the approach to analysis (e.g. machine learning), allowing medicinal chemists to explore previously uncharted territory for the discovery of new drugs. The development of serial crystallography, and the consequent ability to determine structures at room temperature, will complement the unique opportunities to explore dynamic processes offered by XFELs. The engineering of beamlines to operate entirely in vacuum will provide orders of magnitude improvements in signal to noise, and the construction of the next generation of microfocus beamlines will allow structure determination from sub-micrometre crystals.

The provision of these technologies will synergise with the advances in cryo electron microscopy (cryoEM) to finally bring within reach high-resolution analyses of, for example, many membrane proteins of known therapeutic relevance. In addition to molecular-level studies, advances in synchrotron-beamline technologies (tomography, microscopy) will offer unprecedented opportunities to map out cellular and tissue structure at the larger length scales of a few tens of nanometres. These advances will also synergise with those of super-resolution light microscopy and cryo electron tomography (cryoET), making real the prospect of mapping out cells with better than organelle resolution and even entire organs with subcellular resolution.

The ability to seamlessly link data from a full set of imaging modalities on the scale of tissue, cell, sub-cell and molecule, will provide completely new perspectives on the biology underpinning human health and disease. Importantly, the co-location of cryoEM and cryoET facilities with synchrotron beamlines is already cross-fertilizing technology development as well as enhancing user access.

The ability of the European accelerator-based light sources to drive forward these advances as a federated grouping will be greater than the sum of their individual efforts. A commitment to common sample and data formats will allow the scientific community to harness efficiently the full network of LEAPS and, crucially for biomedical research, to pool huge quantities of data to unleash the power of artificial intelligence or machine learning for therapeutic discovery.

Energy



The grand challenges – sustainable production, storage, and use of energy

The scientific answers – new materials as well as production and storage technologies

The LEAPS role – non-destructive operando imaging and spectroscopy of realistic devices to optimise materials and processes

The LEAPS impact – smart specialisation across facilities and development of new spectroscopy and imaging methods based on increased source brightness

Sustainability is a key factor in accommodating the growth of the world's population and its future demand of resources for water, food and energy, all of these at a higher standard of living for the average citizen. This requires a significant change of today's practices, including the minimisation of footprints in materials' manufacturing, but also use during the products' life cycle and clever reuse of the material or its components. Both the production and storage of energy represent immediate challenges to a global population that is consuming nearly 150.000 TWh/year (or 80 GJ/person/year), a number that increases by approximately 10 % per decade. Fossil fuels (oil, coal, and gas) continue to dominate, accounting for over 90 % of energy resources. Renewables, however, are playing an increasingly important role. Integral sustainability must become a driver for new energy technologies, for creating durable systems to produce, convert, and store clean energy.

While initial efforts have been aimed at reducing the footprint by making existing technologies more efficient, the final goal is a (circular) society based on truly sustainable resources for energy and materials. In this transition to a sustainable society, advanced materials will play a crucial role. These will have the following in common: less non-renewable energy use and less greenhouse gas emission during the synthesis, construction, processing, packaging, transportation, usage, recycling and reuse. In order to replace scarce raw materials, functionality must be understood in all its detail. Further development and increased availability of techniques using accelerator-based light sources is a prerequisite in this domain.

Currently, 85-90 % of the chemical products manufactured in industry rely on the use of catalysts in one or more stages of their process.

Moreover, the importance of catalysts in the field of energy continues to grow. The chemical sector aspires to be increasingly active along the entire value chain from feedstock to end-user market and therefore research and development in catalysis is crucial. At the same time, societal issues and legislation call for a shift towards new energy carriers (hydrogen, electrons, chemicals), using alternative energy sources (e.g. solar) and feedstocks (biomass, CO_2), as well as energy and atom-efficient processes. Any advances in catalysis will require optimal control over chemical reactions, and a fundamental understanding of the role of catalytic sites and surface structures. Such insights in catalyst performance, at all the time and length scales of the reaction, will help in the design and development of catalysts in a bottom-up approach.

Conduction and storage of electricity, heat and hydrogen are the most important challenges to solve the energy problem faced by society. Notable progress has been made, in particular regarding lithium-ion batteries, not least through a deeper insight of cycling and long-term degradation from operando studies using parallel and complementary X-ray techniques.

Batteries are just one way of storing energy. Another approach is to convert excess renewable energy into chemical bonds. It is envisioned that we will need a palette of solutions, including direct solar-to-fuel devices, photovoltaic/electrolysers and fuel-cell technologies, in addition to efficient batteries. Key factors here are efficiency, stability and costs. Flywheels and batteries, for example, are too expensive to be considered for seasonal storage, while chemical storage is too inefficient for storage shorter than (typically) a day. A viable solution for the storage of excess renewable energy may be the use of electrolysers. Current electrolysers have a maximal efficiency of 70 % and are based on noble metals such as platinum and iridium. Large-scale applications are only possible if more abundant electrode materials are developed, probably based on base-metals, and also if the efficiency of electrolysers can be improved. Renewable hydrogen can then be used to convert CO_2 to fuels. The challenge is to develop both cheap materials for photoabsorption and catalysis and then to integrate those in a device with an overall solar-to-hydrogen efficiency of at least 20 %. This will require a detailed understanding all along the process chain.

Future breakthroughs require a knowledge-driven approach to achieve a fundamental understanding of material quality, chemical (from atomic to surface to bulk) and mechanical interactions, and the effect of scaling to industrial outputs. Market penetration can only succeed if materials are designed which remain inexpensive, exhibit high efficiency, and have a low environmental impact throughout their life cycle. It seems probable that nanotechnology and the novel properties associated with an increased surface-to-volume ratio will play a decisive role in achieving the required paradigm shift. Investigations and comprehensive screening of such systems will necessarily be based on multiscale studies most effectively pursued using multiple and parallel synchrotron and FEL techniques such as X-ray tomography, spectroscopies, and scattering methods such as small and wide angle scattering, and total scattering, on true operando systems; i.e. multidimensional studies probing different length and time scales characteristics, parameters, etc. A key factor for success will be advanced data processing and analysis methodologies, including artificial intelligence, in order to analyse and interpret these large amounts of data. Synchrotrons and FELs in the LEAPS collaboration will act as hubs between academia and industry in this urgent challenge of characterisation, analysis and interpretation.

Environment

The grand challenges – Understanding and mitigating the anthropogenic impact on soil, water, air, and the climate

The scientific answers – Understanding molecular reactions in real time of relevance to ecology, sampling molecules and trace elements in the eco system

The LEAPS role – Spectroscopy of highest sensitivity and specificity to identify specific molecules and trace elements and to follow them in chemical reactions

The LEAPS impact - Europe-wide coordination and standardisation allowing researchers to measure samples with many techniques and compare very large number of samples measured at different LEAPS facilities.

The anthropogenic impact on the environment in the 21st century includes global warming, oceanic acidification, an increased imbalance in the carbon- and nitrogen cycles due to deforestation, unchecked agricultural practices, and myriad forms of pollutants introduced into the air, soil and water reserves, and difficult-to-predict strains on natural resources such as clean water. Many of the responsible processes involve particles on the molecular or nanoscale that can, in addition, be highly diluted but nonetheless remain potent agents of damage. Examples include fluorocarbon-based aerosols, microbeads, carbon monoxide, and micrometre-sized particulate matter, including plastics.

The solutions to these challenges are very diverse and range from the use of catalysts to microbes and organisms to remove pollutants such as heavy metals from soil, capture and convert CO_2 from the atmosphere, or break down plastics in the oceans.

A complete understanding of the detailed interactions of any of these systems with their surroundings thus requires statistically relevant studies of real-life systems using microscopic probes with intensities sufficient to detect often very low concentrations of material. The tunability of synchrotron and FEL radiation and the much-increased brightness and spatial resolution offered by the new generation of synchrotrons and FELs that will dominate the LEAPS programme will be critical in attaining these goals and providing novel solutions based on this information.

The techniques that can be employed in X-ray environmental studies range from the low photon-energy regime (such as spectro-microscopy of low-Z elements) to the high-energy methods such as X-ray absorption spectroscopy, ptychography, X-ray diffraction, studies that can be performed either in the static or ultrafast modes, and total scattering. Single particle imaging is possible in the case of FELs. The LEAPS programme should be the basis for a Europe-wide coordinated effort based on smart specialisation. The large number of samples that will need to be investigated will require the standardised implementation of robotics, massive data handling, and machine learning, all of which are being developed and refined at accelerator-based photon sources.

Food security

The grand challenges – antibiotic and herbicide resistance; soil, crop and animal health

The scientific answers – novel fertilizers, herbicides, veterinary drugs and vaccines

The LEAPS role – leveraging advances in brightness, automation and computation to generate new chemistry and biotechnology

The LEAPS impact – Europe-wide exchange of technological know-how and coordination for common formats for sample input and data output

Many of the issues and opportunities discussed in the context of human health and the environment are equally relevant to food security in the 21st century. The last century saw major advances in agricultural productivity underpinned by scientific research that had yielded improved fertilizers and herbicides and well as antibiotics and vaccines. These advances are now threatened by the rise of antibiotic and herbicide resistance. The widespread use of chemicals, and intensive farming methods, has generated unanticipated challenges such as the loss of pollinators. Shifts in global climate conditions pose risks from viruses new to European livestock (e.g. the bluetongue virus). Soil health and aquatic populations are threatened by pollution ranging from leaching to packaging and nanoparticles. Biofilm formation by microbes poses major challenges for food-processing industries.

As in human healthcare, new therapeutic agents and vaccinology strategies will be required to meet the challenges of maintaining a healthy livestock population. Novel chemical processes will be needed to provide new agrochemicals as well as methods to combat pollution. As discussed earlier, multiple advances in technology for X-ray crystallography beamlines will accelerate the structure-guided design of novel compounds and bioengineered reagents (e.g. designer enzymes with bespoke catalytic functionalities). Microfluidics and nanofluidics will revolutionise sample delivery at next generation beamlines for screening particulate materials. Advances in imaging, tomography and ptychography will provide a completely new toolkit of techniques with which to probe biofilms.

Again, the exchange of know-how and definition of common formats for sample input and data output resulting from LEAPS activities will streamline the translation of scientific results from accelerator-based photon sources into improved food security.

Engineering & manufacturing

The grand challenges – improving efficiency of existing and discovery of novel and smarter materials and fabrication techniques, reduced environmental footprint

The scientific answers – design, synthesis, and characterisation of new materials and their combined synergistic applications, advanced manufacturing (e.g. 3D printing)

The LEAPS role – imaging, diffraction, and spectroscopy to understand physicomechanical properties over several length scales

The LEAPS impact – improved photon beams and sample environments provide better insight. Smart specialisation between facilities provides optimised and coordinated portfolio of techniques

Engineering and manufacturing affect virtually every aspect of our daily lives, from urban infrastructure (e.g. civil engineering, energy generation and provision, and transport), via food, health and the environment, to high-tech products in the electronics and medical branches.

Many of the breakthrough developments in all these fields have come through insights and discoveries in materials science. Accelerator-based light sources have played a leading role in materials investigations and through this innovative design in both fundamental bottom-up and pragmatic top-down approaches. These have varied widely, from investigative studies of composite architectures and structures using 3-D imaging (e.g. through absorption, phase, diffraction, and chemical tomography and ptychography), often taking inspiration from nature and its uncanny ability to produce structures that manage to combine lightness, frugality of bulk, and strength in the field of biomimetics; to microscaled in situ and time-resolved diffraction studies of fabrication processes, most recently in attempts to optimize the solidification mechanisms in 3D printing and other additive-manufacturing processes, to name just one example. Moreover, the performances of well-established materials, such as concrete, or containment materials in nuclear facilities, have undergone significant improvements by insights into chemical and mechanical degradation factors and during life-cycles. A recent field, which is expected to grow because of industrial demands is battery research. In this manner, sea-changes in engineered objects via smart combinations of two or more materials in controlled architectures and their macroscopic formation of hitherto impossible structures across the entire gamut of engineering and manufacturing, including the aerospace and automotive industries.

The orders of magnitude improvements in coherence, brightness and pulse length promised by the LEAPS facilities will be game-changing in these fields. Phase contrast and lensless imaging, pivotal in investigations of complex but often only subtly heterogeneous systems, will benefit hugely by the increased coherence fraction, thus providing nanoscale data on macroscopic objects up to the centimetre scale.

Chemical and diffraction line tomographies, as well as microdiffraction, will likewise yield hitherto unimaginable insights into real and complex engineered systems and their future improvements, so urgently required in our rapidly developing society.

The ability of the LEAPS facilities to provide dedicated experimental facilities to a variety of these problems via smart specialisation will open a whole new door for European industry. To exploit the full potential of these techniques requires coordination and optimisation from the source, over the experimental environment, detectors to the data analysis and even to the access rules. Only coordination between all facilities to implement one common technology roadmap and agree on European-wide standards for collaboration with industry can secure the potential of these tools for the much-needed development in engineering and manufacturing.

Heritage science

The grand challenges – understanding the human culture and development

The scientific answers – investigation of palaeontological objects and human artefacts

The LEAPS role – imaging and spectroscopy to understand origin, fabrication and conservation of unique precious objects

The LEAPS impact – standardised measurements and reference materials allowing systematic studies and comparisons. Smart specialisation giving all access to the few specialised beamlines

Heritage objects from archaeology, palaeontology and the arts provide essential information about our history, culture and society. A first set of research questions regards the origin of heritage materials, and the necessity of understanding their history, their manufacturing background, their transmission, the political, cultural or symbolic uses they represent, and their alteration over time. A second set of questions concerns the diagnosis of the current state of heritage materials in objects. A third set concerns their future: their conservation, restoration, and transmission to our own and future generations. For instance, a work of art is a dynamic object that from the moment it is created is subject to chemical and physical changes that ultimately results in an altered and degraded appearance. Ageing effects on works of art are obvious (changes in colour, surface crust or corrosion formation, mechanical failure, etc.), but not very well understood; neither are the methodologies to clean and preserve them. For instance, in many of Rembrandt's paintings, including "The Night Watch" (1642), whitish, insoluble crusts cover smalt-rich paint passages as a result of components migrating out of the paint to the surface. It is not known to what extent solvent-based cleaning treatments would exacerbate the degradation of these paints.

All these scientific questions are particularly complex. Indeed, heritage materials are not model materials for which the analytical parameters are known a priori. Many internal as well as external factors play a role. The internal factors, such as the material composition, are mostly highly complex as they are heterogeneous systems. In addition, environmental factors such as burial conditions in archaeology and palaeontology, exposure to light, fluctuations in temperature and relative humidity, airborne pollutants, as well as human intervention due to restoration treatments undertaken during the object's lifetime accelerate the degradation process. The history of the objects is often largely unknown.

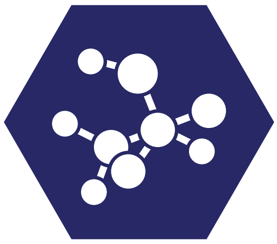
Often only very limited information on previous cleaning and conservation procedures is available. To understand degradation processes, it is important to retrieve as much as information of the art objects as possible, with the right balance between the information sought and impact of the measurement.

Spectroscopy and imaging provided by accelerator-based photon sources play a major role by providing complementary means to investigate the heterogeneous physical and chemical nature of samples and movable artefacts.

For instance, 2D X-ray and UV/visible spectral imaging and 3D micro-tomography provide critical information to decipher the manufacturing process of archaeological artefacts. The same set of methods is instrumental to infer taxonomy and life environment of the most important fossils stored in natural history collections.

Europe is a worldwide leader in the field and currently develops E-RIHS (European Research Infrastructure for Heritage Science), which will contribute to establishing a tighter link between Heritage Science and facilities, ideally via LEAPS.

Fundamental science



The grand challenges – understanding the universe we live in

The scientific answers – new insight into fundamental science as well as methods and tools to broaden our horizon

The LEAPS role – state-of-the-art imaging, diffraction, spectroscopy tools and methods being made to all areas of natural science

The LEAPS impact – coordination and exchange between LEAPS facility to maintain the European leadership and push the field forward

If "Information is the new oil" that makes modern society evolve and move, knowledge is an inexhaustible oil field. Fundamental science is about widening our understanding of planet Earth and of the universe around it. A better comprehension of physical, chemical, biological laws always benefits the direct research meant for health, energy, environment, IT, industrial progress. Synchrotron and FEL generated radiation plays both a direct and an indirect role in the "oil" game.

Directly, X-ray techniques are outstanding tools for fundamental science: atoms, molecules, liquids and solids can be probed to their core properties, theories can be tested with great accuracy, macroscopic behaviours can be explained by microscopic phenomena. Moreover, the sensitivity and penetration of X-rays allow studies on tiny portions of matter brought to extreme values of pressure and temperature, otherwise unreachable in the lab but common inside the Earth and other celestial bodies. For example, static and dynamic X-ray spectroscopy and diffraction will be used on sub-micrometre sized samples, reaching pressure values typical of the core of Earth, providing information about structure, sound velocity, and magnetisation that are needed to formulate better models of Earth and other planets. Synchrotron and FEL radiation are great direct enablers of fundamental scientific progress.

Indirectly, research in fundamental science has been the driver of technological progress in synchrotron and FEL sources. Experiments in basic science are constantly pushing the limits of technology, refining existing methods and inventing new ones, opening new opportunities for more applied work. Researchers in fundamental science have been the fastest to profit from better synchrotron and FEL sources, and are often those with the most demanding requests to facilities. The subsequent benefit for the user community has been huge and widespread. For example, energy loss spectroscopy with X-rays started as a technical challenge motivated by the need to test models of sound in liquids.

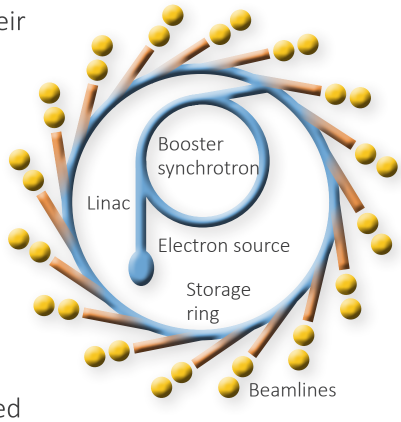
Later it developed into an accepted method to determine lattice, magnetic and charge excitations in materials of fundamental theoretical interest; in future synchrotrons and FELs the technique will be more accessible and will become an advanced characterisation tool; meanwhile, the same technologies are being applied to enhance by orders of magnitude the sensitivity of more widespread spectroscopies (e.g. X-ray absorption) currently used for catalysis, environmental, energy and biophysics studies.

Excellence in synchrotron and FEL radiation is boosted and gauged by the quality and novelty of fundamental science conducted at facilities. Competition and fair collaboration among European synchrotrons and FELs must be kept at the highest level to preserve the recognised leadership of our network in almost every field. LEAPS can help coordinate efforts across the continent, directing special resources where and when they are needed and ensuring that outcomes become beneficial to all partners. Examples are the development of X-ray detectors, optical components, mechanics, and data-analysis tools. In fundamental science, excellence and flexibility are more important than standardisation and ease of use, and adequate resources must be provided in the future years.

Fundamental science is constantly advancing the frontier of technology; a dynamic synchrotron and FEL radiation network will stimulate the European industry to develop innovative products, often in collaboration with LEAPS facilities that can be later transferred to larger markets, thus helping Europe in the global competition of information and manufacturing industry. In addition, they will themselves develop methods and techniques that can be passed on to European industry enhancing their competitiveness.

What is a synchrotron light source?

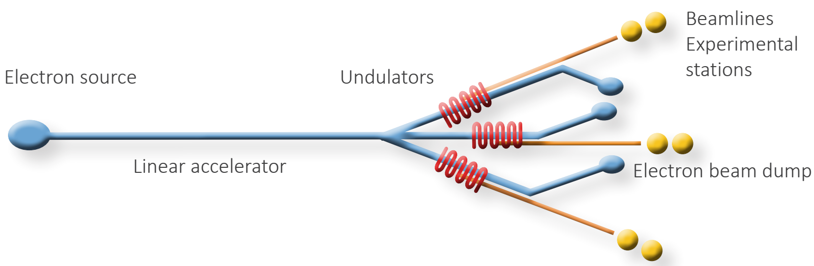
A synchrotron light source is made up of several key components: a source of electrons, a linear accelerator, a booster synchrotron and a storage ring. Electrons are generated in an electron gun, and accelerated in bunches of several billion in the linear accelerator before continuing their journey into the booster synchrotron where they are further energised. Once the right energy is reached, the electrons are injected into the storage ring where several hundred bunches of electrons race around at just under the speed of light. At various points around the storage ring, these electrons pass through specially designed magnets and emit brilliant synchrotron light. This light is channelled down to the experimental stations, which are known as beamlines. Many experiments can run simultaneously making a synchrotron a high-throughput environment with the ability to support a large community of scientists.



What is a free-electron laser?

Free-electron lasers (FELs) are also accelerator-based light sources, utilising electrons to generate beams of light with unique properties. Unlike circular synchrotrons, FELs are based on a linear accelerating structure.

The electron beam is passed through magnetic undulators up to 300 m long. These arrays of magnets can be manipulated to produce the required light for a given experiment. Through complex interactions between the photons and electrons in the undulator, the electrons arrange themselves into thin disks which emit light in a highly synchronised way. The resulting light from these minute electron disks is pulsed and laser-like. This enables the study of processes at the atomic scale across a range of timescales, reaching the femtosecond, which was previously inaccessible to researchers. Each FEL possesses a number of beamlines enabling research into physical and life sciences.



For further information please visit the LEAPS website or email: info@leaps-initiative.eu

www.leaps-initiative.eu

LEAPS League of European Accelerator-based Photon Sources