NEUTRONS FOR SOCIETY

Science Strategy

June 2025

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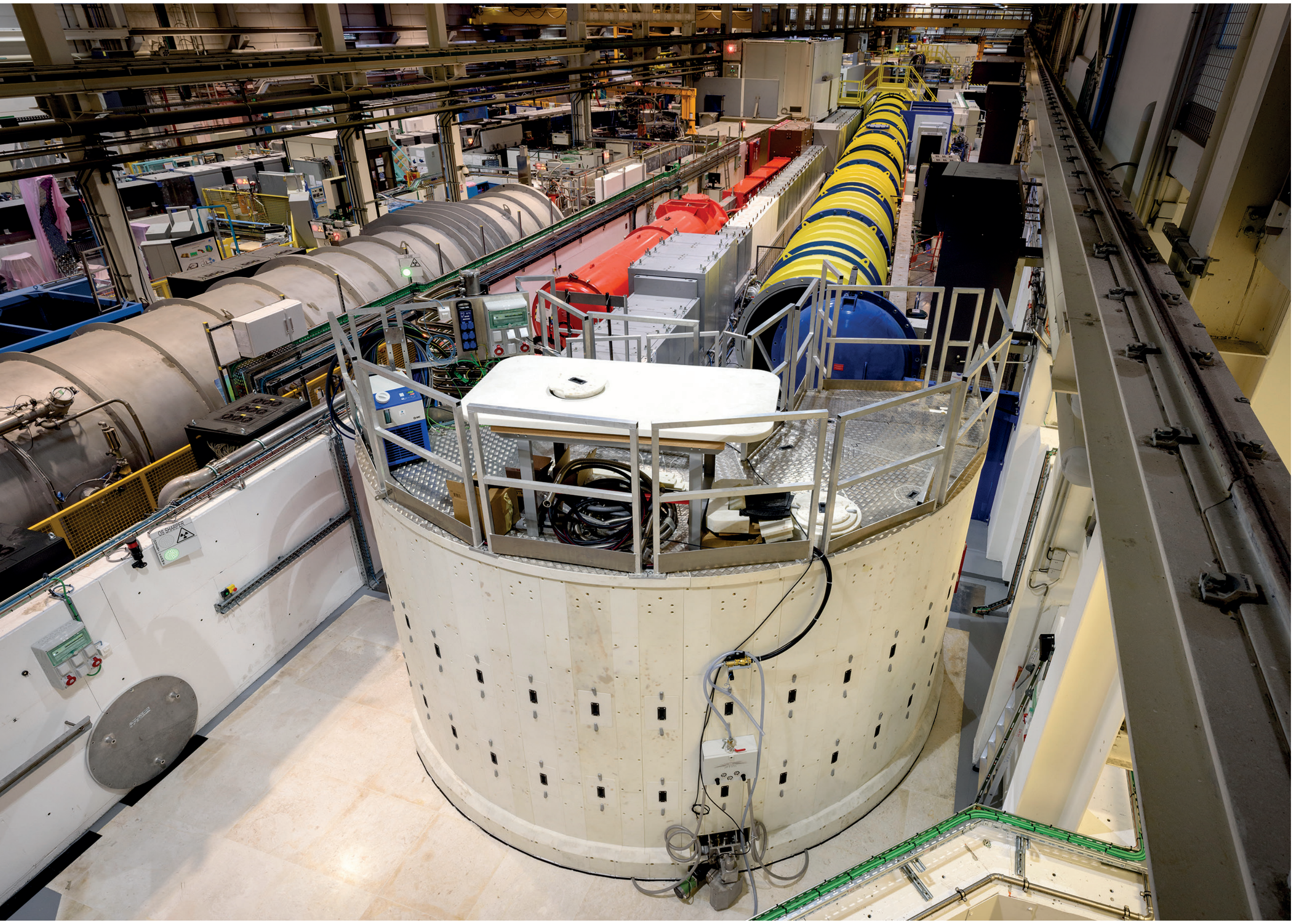

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Executive summary

The ILL Science Strategy outlines the approach that will be taken to leverage the improvements to the instrument suite achieved thanks to the recently completed Endurance programme, with the aim of enhancing our science programme in order to expand our user community and address some of today's major societal challenges. It provides a vision for ILL scientific operation for the coming decade, serving as a guide to ILL leadership on resource allocation, strengthening and demonstrating ILL's importance to European science and innovation, and supporting political decisions on the future European neutron landscape.

The Strategy reflects the need to achieve a balance between the consolidation of existing strengths and the creation of new structures and mechanisms to support emerging scientific areas of societal importance. The scientific excellence delivered by our peer-reviewed user programme will continue to provide the foundation.

In Nuclear and Particle Physics, we will focus our attention on Flagship Experiments – those involving long-term collaborations with external users.

We will create new structures, known as *Science Hubs*, covering the following four areas:

- Quantum materials
- Liquid-liquid phase separation
- Li-ion batteries
- Advanced manufacturing

These will be centres of scientific expertise whose purpose will be to support and expand the user base, promote internal collaboration, boost links with and relevance for industry, and deliver high-profile science. The Hubs will bring together internal and external scientists under the leadership of a prominent scientist, whose task will be to define a 5-year research project and then to coordinate the work of the team to deliver its objectives. The project will be selected by a competitive proposal process and will be peer-reviewed to ensure scientific excellence.

A new mechanism will be introduced to design and perform key Showcase Experiments with the aim of opening up a new field of activity, attracting new users and providing high-visibility societal impact. These experiments will require more resources and longer time scales than regular experiments, but have the potential for higher impact. Three initial topics have been identified:

- Superconducting wires
- Cell structure with high-resolution bio-imaging
- Water membranes for a sustainable future

We will consolidate and expand our programme in nuclear medicine, increasing our production capacity for radioisotopes for cancer treatment and continuing to invest in the development of isotopes for future diagnostics and therapies.

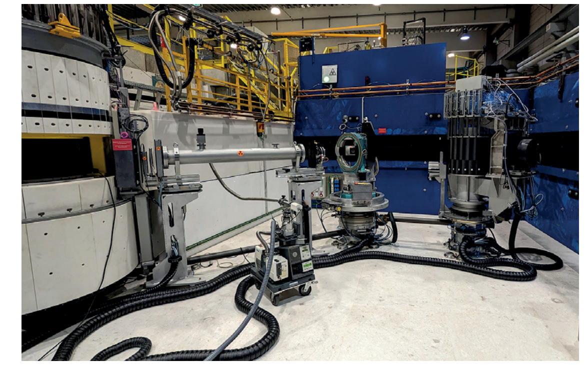
The ILL's PhD programme will be enhanced and partially redirected towards the scientific priorities of the Science Strategy.

Clear scientific needs have been identified to increase our capacity for neutron imaging experiments, as well as to strengthen computing support for experiment planning and execution and for data analysis, including the use of enhanced AI and ML tools. We aim to address these needs through the development of infrastructure and personnel.

A new instrument group for *Applied Science* will include imaging, strain scanning and irradiation instruments, and will have the mandate and resources to strengthen collaborations with industry.

The success of the ILL also relies on the effective communication of its impact. There will therefore be increased emphasis on Communication and Outreach, which will benefit all aspects of the Science Strategy.

ILL Science Strategy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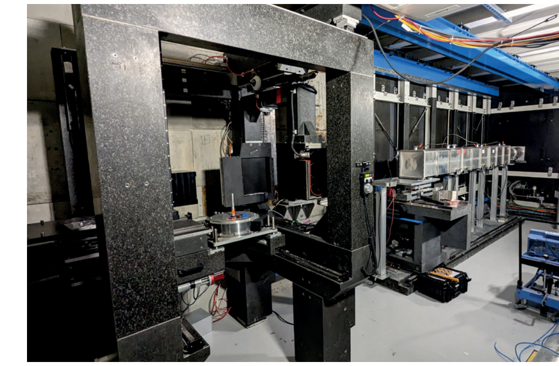
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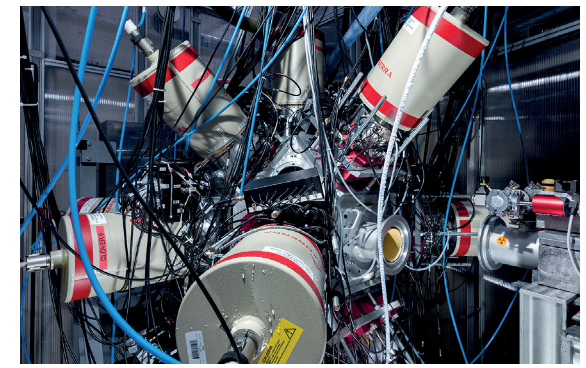
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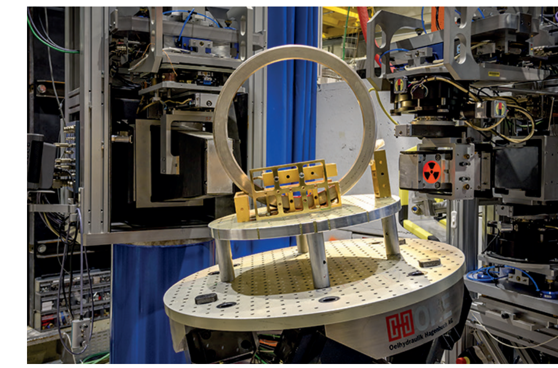
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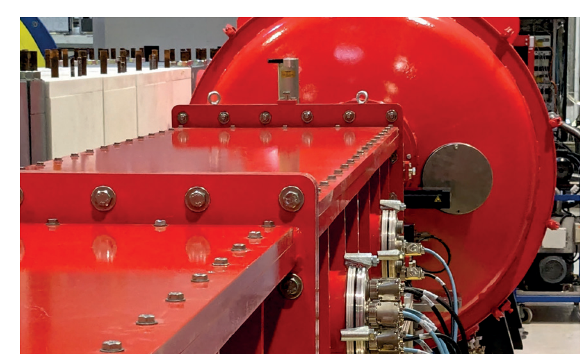
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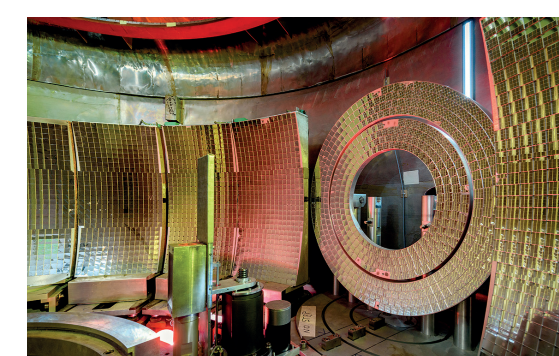
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1 Introduction

1.1 CONTEXT

The ILL has been the leading neutron source in the world for more than 50 years. It has made – and continues to make – essential contributions to many areas of science of benefit to our society, and has had a huge impact on science and the scientific community. Over its years of operation, the ILL has developed and set the gold standard for running a user facility for the scientific community.

The institute recently completed a major series of upgrade and expansion projects to its suite of neutron instruments through the Endurance programme. It is also in the final stages of renewing the neutron source, ensuring continued compliance with the highest safety and security standards. The conclusion of these projects sees the ILL at the peak of its performance, operating the largest instrument suite of any neutron facility and capable of performing an unparalleled range of world-leading science for the coming decade.

The next step is to develop a strategy that capitalises on this position to maximise the impact the ILL has on science and society, particularly in addressing major societal challenges. An aging population, climate change, the need for sustainability, digitalization, and the geopolitical situation all create challenges that require answers from science. Large-scale research infrastructures can provide major contributions. In Europe, the particular task for all research infrastructures is to establish themselves at the frontier of excellence and accelerate innovation, thereby contributing to delivering European economic growth[1].

The ILL has taken this opportunity to re-evaluate how it supports science and its impact on society, aiming to think creatively in order to identify opportunities for improvement. The initiative addresses key recommendations from an *ILL Strategy post 2023 Working Group*[2], set up following the signature of the 6th Protocol to the Intergovernmental Convention. The Working Group recommended, among other things, that the ILL focus on areas of high societal impact both through the implementation of new access models and through the enhancement of in-house science. The ILL Science Strategy document articulates how we intend to pursue those aims. The Strategy leverages the capabilities created by the completion of the Endurance programme and will provide a foundation for ILL operation for the coming decade.

1.2 OBJECTIVES OF THE STRATEGY

The Science Strategy will serve as the basis for a plan on how to maximise our scientific output and societal impact while continuing to strengthen our user community and enhance user support. It will allow the ILL to demonstrate its importance to European science and innovation within our operating horizon and to support political decisions on the future European neutron landscape.

The Science Strategy will serve as a guide that ILL leadership will use to make decisions on resource allocation. The document itself will serve as a communication tool to strengthen and disseminate the ILL value proposition. The Science Strategy will also reinforce recruitment and retention by strengthening our scientific culture.

The Strategy must reflect a balance between the consolidation of our strengths and the development of emerging scientific directions. The goals that it outlines must be achievable within a relatively short time, of the order of a few years, and its content and implementation will need to be reviewed and updated periodically.

The Science Strategy aims to describe:

- The existing strengths of the ILL that will be continued and supported, in particular through the regular user programme.
- Scientific priorities in new and emerging fields, as well as in existing areas that will be consolidated and reinforced. The priorities are supported by narratives and examples to demonstrate their potential short- and medium-term impact on societal issues.
- New implementation mechanisms and structures which will be put in place to achieve the aims of the Science Strategy. Science cases to justify the goals of the new mechanisms will be defined as part of their implementation processes.
- An indication of the resources and infrastructure needed to support implementation of the Strategy
- An integrative approach for communication, external funding opportunities and stronger connections to industry.

1.3 THE STRATEGY DEVELOPMENT PROCESS

The process began in early 2024 with the setting-up of a Science Strategy Working Group comprising 26 members, with ILL and external scientists in equal proportion. The external members were selected from a list of eminent scientists in their fields from both academia and industry, which was compiled with substantial input from the ILL Scientific Council. The selected members represented a diverse range of fields, some of which were and some were not currently addressed by neutron science, and a deliberate effort was made to invite non-neutron experts so as to ensure a fresh perspective. Specialised neutron expertise was provided by the ILL scientists.

The Working Group met several times over a five-month period starting in March 2024, during which time it subdivided itself into five focus groups:

- Digitalization / Quantum Materials
- Universe Essentials and Cultural Heritage
- Health and Life Sciences
- Energy
- Environment and Sustainability

The focus groups identified emerging scientific areas with high priority. They suggested possible resources and mechanisms for implementation, and they proposed potential metrics for scientific output and societal impact. They also highlighted areas of existing strength that should be consolidated or leveraged to further enhance impact. Their findings were assembled into a recommendation report which was delivered to ILL Management on 26 July 2024. The recommendations were the subject of a careful evaluation by ILL Science Management, who made selections from the report for incorporation into the Science Strategy.

The rationale behind the choices made by ILL Science Management can be summarised as follows:

- Some emerging scientific areas were felt to be addressable directly within our existing user programme, requiring only minor adjustments to existing activities such as improved outreach and better follow-up of new user groups.
- In some cases, more substantial changes are needed to maximise the potential impact, requiring the establishment of new implementation mechanisms and access modes. These changes include the creation of Science Hubs and Showcase Experiments, as explained in section 1.4.
- Some areas require investment in new instrumentation or data science capabilities.
- Enhanced communication and outreach were identified as critical in many areas.
- Some recommendations represented challenges to our business model, such as providing more access to researchers based in countries that do not contribute to ILL costs.
- Some recommendations were felt to require prohibitively high levels of investment or expansion of expertise.
- Some recommendations did not meet the criteria for high impact within a reasonable time frame.

All the activities covered by the Science Strategy will be reviewed regularly, and the Strategy may be modified following a critical assessment of its progress. Scientific excellence will remain our key driver and will be overseen by an external-peer review leveraging our existing College-based system.

1.4 NEW MECHANISMS

The science programme at the ILL is currently organised through two administrative structures: the Instrument Groups and the Colleges. The Instrument Groups are part of the ILL organisation chart, with instruments and their corresponding scientists organised according to similar experimental techniques. This organisational structure facilitates the consolidation of technical requirements for instruments and methods of running experiments. The science performed at the ILL is organised through its user programme and proposal system, which relies on the Colleges and their corresponding panels of external experts. The College peer-review system addresses all the types of science performed at the ILL and provides a highly flexible, effective and responsive mechanism to deliver scientific excellence.

The structure of the ILL successfully accommodates great diversity in scientific research and the available neutron instrumentation. However, a consequence of the structure is that ILL scientists can become constrained to a limited range of techniques. This produces specialised experts who provide excellent user support, but can hinder collaboration between ILL scientists despite significant scientific overlap, impacting efficiency in assisting external groups in their research and in offering encouragement to take advantage of complementary neutron techniques. A coordinated, collaborative knowledge base at ILL would increase efficiency in communication, research strategy, and data interpretation for external users.

Consequently, the Science Strategy includes the introduction of two new mechanisms to facilitate external outreach and internal collaboration: Science Hubs in areas where the ILL is currently strong, and Showcase Experiments in fields where the ILL has less experience but where neutrons have the potential to make a significant new impact.

1.4.1 SCIENCE HUBS

We will establish a small number of Science Hubs focused on strategic scientific themes. These Hubs will serve to expand the user base while promoting internal collaboration between ILL scientists.

The Hubs will not compete with the regular user programme but will be designed to complement it. The expertise and communication networks managed by the Hubs will be developed with a mandate to serve the constantly evolving wider user programme. Unlike the ILL Colleges, the Science Hubs are not intended to cover all areas of science addressed at the ILL. Each Hub will serve as a network of scientific excellence and a pole of attraction in a particular scientific area, coordinated by a high-profile scientist and reinforcing internal expertise with external collaborators. Hubs will provide increased visibility and serve as a portal to facilitate outreach to external groups and expand our user community. By drawing on the substantial internal expertise already present within the ILL, it should be possible to set up a successful Hub relatively quickly and economically.

Each Science Hub will have a well-defined research objective within its scientific area, structured as a project with a well-defined set of key performance indicators and a timeline. It will be matrixed across the Instrument Groups and Colleges and will focus, coordinate and consolidate the personal research efforts of ILL scientists across the organisation. For each Hub, a Science Hub coordinator will be selected through a recruitment process open to both internal and external candidates. As head of a matrixed organisation, Science Hub coordinators will not have line management responsibility, and will report directly to the Science Director. Their primary task will be to define and coordinate the execution of the research within their Science Hub and stimulate the scientific life of the staff who choose to join the Hub. Science Hub coordinators are expected to be closely involved in the ILL user programme and, to this end, should be closely integrated into the experimental teams directly linked to the Science Hub topics.

As part of the selection process for the positions of Science Hub coordinator, each candidate will be required to prepare a proposal for a research project structured around specific objectives and performance indicators and supported by a strong science case within the relevant scientific area.

The projects will run for five years and will be reviewed every two years. The research projects selected will be presented regularly to the Scientific Council for advice and to report on progress.

Vision and expertise in the relevant sub-field are clearly prerequisites for a successful Science Hub coordinator. Just as importantly, the coordinator must have a collegial attitude allowing them to attract sufficient ILL staff to commit to the Hub to create an efficient collaboration for rapid and impactful results. Applicants will be expected to estimate the internal resources required to achieve their proposed research objectives, preferably with an identification of the ILL staff who are likely to join the Hub.

Each Science Hub will receive a recurrent budget, floor space, capital investment for equipment and dedicated PhDs/post-docs. Support may include time and resource commitments from other groups within the ILL (e.g. computing, technical, design, engineering). The Science Hub coordinator will commit to regular meetings and effective coordination, and will be strongly encouraged to seek external support, such as through national, EU (e.g. ERC) and international grant applications and through collaborations with universities and industry. The Science Hub may acquire and oversee equipment critical for advancing their scientific area, which will be made available to the user programme. This could include tools tailored to characterising the samples required for neutron studies, using both ILL and external financial support.

ILL scientific staff will be invited to join the Science Hub that matches their scientific interests, and would be required to commit a reasonable fraction of their personal research time to the Hub. The incentives for staff to join the Science Hubs include gaining access to the additional resources made available for their chosen areas of interest, being part of a wider collaboration with support from their colleagues, and benefitting from the leverage both within the ILL and in the external community for additional resources and infrastructure support. The aim is to develop a critical mass that makes the Hub an effective and efficient force in its field for the benefit of the user community. A well-run Hub will promote the ILL as a centre of expertise in the relevant field, attracting attention and external users and collaborators.

We currently plan to launch four Science Hubs in different fields. Their starting dates will be staggered in time based on the resources available, and to allow lessons learned from the first Hubs to benefit subsequent Hubs. Future reviews of the Science Strategy may add or remove Science Hubs.

1.4.2 SHOWCASE EXPERIMENTS

The Science Hubs will be complemented by a small number of Showcase Experiments. The purpose of Showcase Experiments will be to open up a new - and potentially risky - field of activity in order to attract new users and hence expand the range and impact of the ILL.

Whereas Science Hubs leverage an existing critical mass of scientific expertise within the ILL, Showcase Experiments can target areas where the ILL, and more generally neutrons, have limited experience and current impact. Their scientific success may therefore depend on successfully connecting with motivated external groups. The external user group will need to work closely with ILL scientists and other staff to develop and execute the experiments. In that sense, they are similar in spirit to the experiments performed within our existing user programme, but they stand out because of their greater resource requirements, longer time scales and potentially higher impact.

We expect the timescales for developing and executing Showcase Experiments to be of the order of two years. In each case, a team consisting of internal and external members will be assembled whose initial task will be to write a Showcase Experiment proposal, which will be evaluated through a review process to ensure high quality and compliance with safety rules. The proposal can include requests for staff, equipment and multiple periods of beam time over the duration of the project.

Showcase Experiments are intended to address high-risk high-reward opportunities and open new areas of science and societal impact. They aim to show a proof-of-concept or a textbook example for how the ILL's technical capabilities can be beneficial in addressing an important societal question. They will be accompanied by strong external communication focusing both on the broader themes as well as on the accomplishments of the individual experiments.

The process will start with a call for Showcase Experiment proposals, specifying the three topics presented in the current document. We envisage that further calls for proposals will be opened later, as we gain experience in the process.

2 Existing strengths of the ILL

It is important that the Science Strategy not only identifies new areas and approaches to be pursued, but also examines and effectively leverages the existing strengths of the ILL. This section specifically addresses this aspect.

2.1 USER PROGRAMME, COLLEGE STRUCTURE, BEAM TIME ALLOCATION

- The user programme will not significantly change.
- The national balance and 2/3 rule will be maintained.
- The access modes will remain largely unchanged, with a global average of ~80% of the available beam time offered to the user programme.

The Science Strategy will not significantly change the current user programme or the college structure. The ILL's user programme is based on a system of open proposal rounds, in which scientific excellence is ensured by external peer-review organised into a set of science-themed subcommittees known as Colleges. Though continually adjusted over time, the basic functioning has remained largely unchanged for 50 years. It consistently delivers high-impact science and has proven itself to be highly effective in responding to the evolving needs of the external scientific community. It has served as the model for other large-scale research infrastructures, and similar programmes can be found at all the major neutron and light sources in operation today.

We will maintain the current system of *national balance* in which proposals are judged exclusively by scientific merit and small adjustments are then made to ensure a fair allocation of beam time in proportion to the financial contributions of the individual countries to the ILL budget. We will also maintain the 2/3 rule in which beam time allocated through the user programme are heavily biased towards those proposals with at least 2/3 of the proposers' affiliations from countries that fund the ILL. These two elements are essential aspects of our business model. Departing from them would undermine the motivation for countries to pay for Scientific Membership of the ILL.

The Science Strategy intends to maintain the current *80-20 split* between access modes. The user programme allocates 80% of the total available beam time to the highest-rated proposals, while the remaining 20% is labelled as in-house beam time, which is used for a variety of other purposes: Some is set aside as buffer time to compensate for lost beam time in user experiments and thus effectively returns to the user programme. Some is used for commissioning, calibration and test experiments. Some is used for in-house science, and some is used for external users through other *access modes* such as *Easy Access* for rapid-access experiments using standard sample environments and *Director's Discretionary Time* for high-profile time-critical studies. While the new Science Hubs and Showcase Experiments will need some dedicated beam time, we do not expect this to affect the basic 80-20 split. With the completion of Endurance, the reduced need for commissioning time will directly benefit these new structures within the 20% of beam time allocated outside the user programme.

The recommendations from the Science Strategy Working Group identified and highlighted many important existing and emerging scientific areas with high visibility and societal impact, ranging from fundamental knowledge in quantum materials and magnetism, structural biology, biophysics and soft matter, to more applied problems such as fuel cells, thermoelectric materials, photovoltaic materials, nuclear fission, and green concrete and cement. These and other topics will continue to be served by the user programme, benefitting from our existing system of internal scientific and technical expertise and supporting resources and the post-Endurance instrument upgrades. They will benefit from enhancements to our user programme foreseen within the Science Strategy in the form of additional capacity and capability in *neutron imaging*, the reinforcement of *data science*, which will include the use of artificial intelligence and machine learning tools, and a stronger programme of communication and outreach. We will strengthen the data analytics on the experiment-to-publication pipeline, which will inform a targeted campaign of post-experiment user support to improve the materialisation of neutron data into scientific publications.

2.2 FLAGSHIP EXPERIMENTS IN NUCLEAR AND PARTICLE PHYSICS

- We will focus the user programme in Nuclear and Particle Physics on longer-term Flagship Experiments, achievable in a 5-10-year time scale, rather than standard proposals.
- We will focus the NPP Flagship Experiments in two areas: the search for new physics at the precision frontier, and the understanding of neutron-rich nuclei.
- Seven specific scientific problems will be addressed in the NPP Flagship Experiments.

The ILL occupies the world-leading position in nuclear and particle physics activities thanks to its capacity to perform ~20 experiments per reactor cycle, its unique capabilities, and the complementarity of the available instruments, allowing fundamental scientific questions to be studied from different perspectives.

Experiments in Nuclear and Particle Physics (NPP) are often structured as long-term strategic research projects involving strong internal coordination between the ILL scientists and the establishment of long-term collaborations with external users, sometimes with a single expert user team. They typically include a long planning phase, the design and construction of dedicated experimental installations financed and supplied by international collaborations, as well as data-taking running over entire cycles. Results from multiple proposals are often collected into a rich data set that becomes a precious resource for future investigations. These experiments may be consolidated under the term "NPP Flagship Experiments", reflecting their unique goals, need for resources, and potentially high impact. We intend to focus the efforts in this scientific area on such Flagship Experiments compared to standard proposals, as they are typically identified with the ILL as a whole and the results are readily publicised to the broader community to increase the visibility of the institute.

A focus on NPP Flagship Experiments does not require specific restructuring or the creation of new mechanisms. The involvement of ILL scientists will continue to be supported by the regular PhD and post-doc programme, and through instrument developments.

We have identified two key scientific areas to optimise the ILL's scientific output as well as its global visibility: the search for new physics at the precision frontier, and the understanding of neutron-rich nuclei.

The NPP Flagship Experiments addressing new physics at the precision frontier will be focused on the following scientific areas:

- Neutrino physics experiments: The upcoming RICOCHET experiment will exploit the unique advantages offered by the ILL to study neutrino physics. The combination of high reactor power with a compact core, access close to the core with only low cosmic radiation background, and the exploitation of highly enriched ^{235}U results in a time-constant neutrino spectrum needed for high-precision, reliable measurements.
- The neutron electric dipole moment (nEDM): The ultracold neutron source SuperSUN provides a spectrum of particularly low neutron energy with an outstanding phase space density, making it possible to conduct compact statistically-sensitive experiments with well-controlled systematic errors. SuperSUN is indispensable for experiments such as the upcoming panEDM to search for a permanent nEDM.
- Decay correlations in neutron beta decay: The PF1B beamline offers the highest cold neutron flux available at an external guide with the highest polarization and the best polarization analysis worldwide. These characteristics are necessary for precision studies of decay correlations in neutron beta decay. The BRAND collaboration has an experimental plan to use PF1B to measure five as yet unexplored correlation coefficients and further improve the precision on six others.
- Acceleration-bound quantum states of the neutron: Neutrons are ideal particles for experimental studies of fundamental quantum states due to their zero electric charge, tiny polarizability and long lifetime. Flagship Experiments to study gravitationally bound quantum states and "whispering gallery" quantum states will exploit the high cold-to-ultra-cold neutron intensities available on the PF1B and PF2 beamlines through efforts such as the qBounce experiment.

Another set of NPP Flagship Experiments will seek to better understand nuclear forces through the investigation of neutron-rich nuclei. These interconnected research fields have a strong impact on other scientific domains, in particular astrophysics, medicine and energy:

- Accurate fission measurements: The measurements of i) fission yields with detailed error budget and ii) correlations between excitation energy and angular momentum in fission fragments have a strong impact on the understanding of the fission mechanism. The FIPPS instrument would benefit from an appropriate fission fragment identification setup to improve sensitivity to weak fission fragments and to energy and angular-momentum correlation measurements, which would open new horizons in the field.
- High-resolution nuclear structure measurements: The ILL is ideally placed to accurately measure energy levels and gamma decay strengths in hard-to-reach nuclear systems, such as those produced in neutron-induced reactions. This has strong implications on our understanding of the nuclear force and its origin from quarks, and allows us to deduce key information on the nuclear shape.
- Nuclear input for astrophysics: Most astrophysics calculations for the understanding of the nucleosynthesis of heavy elements in our galaxy are severely limited by the lack of reliable nuclear-physics input. Gamma spectroscopy provides insights into specific nuclear states relevant for nucleosynthesis processes and the deformation of nuclei at the r-process waiting-points. An important example concerns the astrophysical origin of ^{180}Ta, the rarest isotope found in the solar system. A collaborative effort by ILL, DANCE and NTOF aims to solve this by studying its gamma de-excitations following neutron capture on a radioactive ^{179}Ta target.

The ILL source offers many unique capabilities for nuclear and particle physics that cannot be matched by any other facility in the world. There are numerous other NPP Flagship Experiments with a potentially major scientific impact that would be well-suited for the ILL, but which would take 15-20 years to produce final results. Two high-profile examples are cryogenic nEDM, offering another order of magnitude in precision over panEDM, and the study of neutron-antineutron-oscillations. ILL involvement in such efforts will need to take our operational horizon into account, and may help to support a bid for lifetime extension.

2.3 PHD PROGRAMME

- The PhD programme will continue and will be expanded, subject to the availability of external funding.
- Current access to university groups will be maintained through the open-call proposal system.
- Expansion will provide dedicated support for the Science Hubs.

The ILL runs a popular and successful PhD programme, currently funding typically 8-9 students per year for up to three years. The programme has been run using an open-call proposal system for more than 15 years and has been an essential element of both ILL scientific life and the user programme, creating close ties with external groups and training the neutron experts of the future. It is funded through a combination of operational funding, direct funding through Scientific Member countries, and external funding (e.g. European NEXTSTEP programme). It is further supplemented by co-funding through the university systems of the host countries.

We intend to maintain the PhD programme in its current form and expand its scope, subject to successful applications for external grants, which is part of the mandate for the Science Hub and Showcase Experiment coordinators. The open-call method for requesting project applications will continue to provide the current number of students each year to the external community. Expansion will enable the method to be modified to allow specific requests from the Science Hubs, the Showcase Experiments, or the NPP Flagship Experiments. We stress that all PhD projects must involve a close collaboration with an external university, as the ILL is not an educational facility and cannot award degrees.

3 Priority areas

The Science Strategy Working Group identified a number of emerging scientific areas with societal impact where neutrons, and the ILL, could play an important role. Priority areas were identified and broadly divided into two categories that could be served by either Hubs, where the ILL currently has a foothold which could be expanded with relative ease, or Showcase Experiments, where experience and expertise is currently limited.

3.1 NUCLEAR MEDICINE FOR CANCER TREATMENT

- We will expand and streamline the programme to produce radioisotopes for medical use and fundamental physics experiments.
- We will study mechanisms to produce useful radioisotopes more efficiently.
- This area will require the opening of an additional irradiation tube, the construction of a dedicated hot cell, and additional staff positions.

All nuclear medicine applications rely on the availability of suitable radiopharmaceuticals. The key ingredient of the latter are radionuclides, produced mainly by reactor or accelerator irradiation of a target. Radioisotopes produced by neutron capture are relatively long-lived (days to months) and are in high demand for therapeutic purposes. They can be synthesized centrally and transported to remote labs without excessive decay losses, in contrast to short-lived diagnostic radionuclides produced at cyclotrons (e.g. F-18), which must be produced and distributed locally.

The ILL is currently engaged in the production of radioisotopes for both research and commercial applications. It is particularly active in the commercial production of Lutetium-177 for cancer treatment, for which the high flux of the ILL reactor offers a unique capacity to meet the high demand from pharmaceutical companies. The efficiency of the ILL for this purpose is so great that its production has an impact on the global price of the isotope, substantially reducing treatment costs. The ILL radioisotope production programme will continue as one of the highest priorities of the Science Strategy and will be supplemented with associated fundamental physics experiments to further understanding and to improve radioisotope production.

Once irradiated, the target material must undergo a number of subsequent steps before being useful for a given application. These steps may require access to wet chemistry laboratories and/or physical mass separation to isolate the relevant isotopes, and biochemistry laboratories to attach the isotope to a suitable vector molecule. Use in research and medical treatment requires quality control and nuclear medicine facilities with appropriate accreditation to conduct in-vitro and in-vivo experiments. The EPN campus does not have these facilities and the ILL will not develop them, not least because of the effort required to cope with the large diversity of radionuclides that can be produced at the ILL. We will focus on the irradiation of raw materials, supplying partner laboratories that are properly equipped to handle and prepare the radioisotopes for further use.

The ILL is extremely well positioned geographically to supply suitable partner laboratories. Partners include international laboratories (ISOLDE and MEDICIS at CERN (CH) for mass separation of radioactive isotopes), national laboratories (PSI Villigen (CH) and NCBJ Swierk (PL) for radiochemical separation), and university laboratories with unique capabilities and competences (Atominstitut Wien (AT), Forschungsreaktor TRIGA Mainz (DE), Hevesy Lab at DTU Risø (DK)). Each of these partners operates its own neutron source or accelerator to produce radiotracers and hence has optimised radioisotope separation processes to handle the high-activity samples obtained from the ILL. The relatively long life of the radioisotopes produced by the ILL allows the efficient transport of the irradiated target to the partner laboratory. Figure 1 shows an example of ILL-produced radioisotopes having been prepared and used by external laboratories for a medical treatment, providing an excellent demonstration that a high-flux neutron source like the ILL is most productive when it is embedded in a lively European landscape of medium-flux radiation sources.

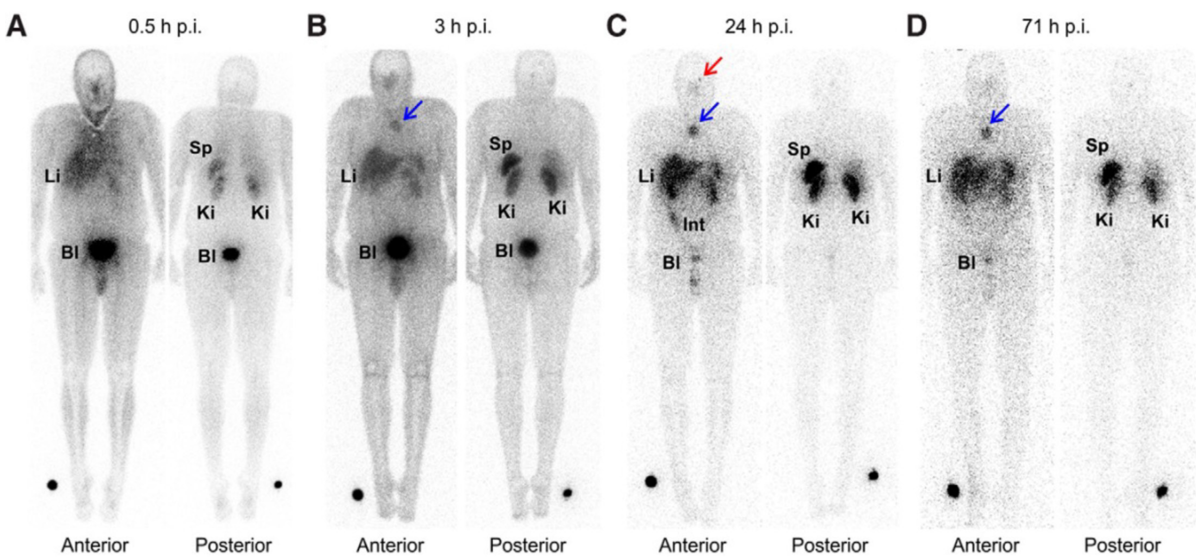

Figure 1: Whole-body images at different time points after injection of ^{161}Tb DOTATOC into a patient suffering from a metastasized neuroendocrine tumour[3]. Enriched ^{160}Gd was irradiated in the V4 irradiation position at ILL, then shipped to PSI to extract radiochemically the ^{161}Tb produced. The purified ^{161}Tb was forwarded to Zentralklinik (Bad Berka, DE) for labelling to the peptide DOTATOC. After quality control, ^{161}Tb DOTATOC was injected into the patient and imaged with a gamma camera to study the bio-distribution over time, a necessary prerequisite to optimise the therapeutic procedure. In total five different labs were involved in this study. © SNMMI.

Radionuclides are needed for medical research, but those produced at the ILL cannot be supplied directly to researchers outside suitably equipped partner laboratories. The ILL is currently embedded in the EU project PRISMAP, the European Medical Radionuclides Programme[4] funded from the Horizon 2020 research and innovation programme, which was created to streamline the process of making radionuclides produced at the ILL and other European facilities available for medical research. This programme includes biomedical facilities with specialised equipment (e.g. dedicated SPECT or PET scanners for small animals), where users can come to perform their experiments in a similar manner to central facilities. The PRISMAP programme mirrors the very successful National Isotope Development Center[5], operated by the US Department of Energy, which pools the resources of laboratories with unique capabilities and competences to make novel, not commercially available, radionuclides available for research projects. The medical research performed with radionuclides supplied by PRISMAP lays the foundations for later commercialisation of radiopharmaceuticals using these novel radionuclides.

PRISMAP is due to expire in 2025, and a follow-up project called PRISMAP$^+$ is under preparation. The ILL will participate in PRISMAP$^+$, which offers the opportunity to discuss with the upstream (target preparation) and downstream (radiochemical processing or mass separation) partners, and sometimes end users, to optimise a process depending on the final application.

PRISMAP and PRISMAP$^+$ address exclusively the needs for medical applications, but radionuclides produced at the ILL can also be used for a variety of other research applications. Examples include the measurement of astrophysically or technologically relevant cross-sections, the measurement of the neutrino mass (HOLMES, ECHo), high-resolution atomic spectroscopy, nuclear probes for time-differential perturbed angular correlation spectroscopy or Mößbauer spectroscopy, and the production of special targets for nuclear spectroscopy experiments at FIPPS. These needs are currently served via bilateral/multilateral case-by-case collaborations.

ILL Science Strategy

The radioisotope production programme will be consolidated and streamlined, involving a restructuring of the current activities across the Reactor, Administration, and Science Divisions. The existing team will be reinforced with an additional nuclear engineer/scientist position and technical support for radiation protection and waste and container-transportation management. To cope with a rapidly rising demand for commercial radionuclides, in particular ^{177}Lu, while maintaining sufficient availability of research radionuclides, a new irradiation tube V6 and a dedicated hot cell for the "decanning" of irradiated samples and loading of shipping containers is to be installed.

3.2 SCIENCE HUB ON QUANTUM MATERIALS

- We will establish a Science Hub on Quantum Materials, which will focus on a sub-topic within the areas of magnetism and superconductivity.
- The Hub will consolidate internal expertise, providing more coordinated support for the external community and rapid responses to emerging problems.
- The Hub will guide the ILL expansion of theory and computational calculation support for the community.
- The ILL will continue to support emerging areas in quantum materials with a strong commitment to the proposal system.

Quantum science and technology are becoming increasingly visible in the public domain, to the point where the United Nations has declared 2025 as the International Year for the subject[6]. Developments in the field are driving innovation and promising solutions to problems that are potentially applicable in many other areas, such as health and energy, and promise to massively improve complex modelling and calculation methods through quantum computing. Research on quantum materials brings together scientists working on a variety of problems at the frontiers of physics, materials science, engineering and computing science. The properties of these systems are uniquely defined by quantum mechanical effects that remain manifest at relatively high temperatures and macroscopic length scales. In turn, these effects can be driven and manipulated to provide novel functionalities and transformative technologies.

Research into quantum materials, particularly in the areas of magnetism and superconductivity, is a historic and fundamental strength of the ILL. The unrivalled ability of neutron scattering methods to probe the length and time scales relevant to the quantum properties of condensed matter is well documented, and the interaction between the neutron magnetic dipole moment and the internal magnetic fields of a material provides a comprehensive and quantitative characterisation of microscopic magnetic structure and dynamics. The science frequently requires extreme conditions, such as sub-Kelvin temperatures, high magnetic and electric fields, and high pressures. Neutrons have low energy, are deeply penetrating, and are electrically neutral, meaning that such challenging experiments are feasible and sometimes even routine. Most importantly, neutron scattering is a quantitative and rigorous technique for measuring the Response Function, which is a mathematical description of the atomic and magnetic structure and dynamics in a sample. The Response Function can be calculated directly from the Hamiltonian, which describes the energies of a physical system. The development of an appropriate Hamiltonian for a material allows all its physical properties to be calculated and predicted, including heat capacity, magnetisation, electrical and magnetic transport, and phase transitions. Neutron scattering is therefore a direct means of testing the validity and limits of the Hamiltonian for a compound, giving unambiguous evidence that is unparalleled using any other method. It is a unique and critical technique for testing and understanding quantum materials.

The research performed at the ILL is rich, diverse and impactful, serving a strong user community. The current user programme serves the quantum magnetism community exceptionally well, providing a highly flexible, effective and responsive mechanism for focusing on the most relevant scientific questions. On average and consistently, just over 30% of the proposals submitted to the ILL over the last 10 years deal with subjects in magnetism, and a similar percentage of ILL scientists specialise in this field. The ILL is particularly well suited for these experiments, with a number of instruments optimised to measure magnetic structures and dynamics covering complementary length and time scales and with a suite of sample environments suitable for studying materials at their quantum limit. The availability of polarized neutrons on numerous instruments, and the expertise in using them, is a particular strength of the ILL, providing unambiguous separation of different contributions to the scattering and on magnetic moment sizes, distributions and fluctuations. Notable achievements include the characterisation of spin ice[7], flux line lattices in superconductors[8], topological magnetism in Weyl semimetals[9], resonances in unconventional superconductors[10], and textbook examples of quantum magnetic fluctuations[11]. We strongly support the science in these areas and will continue to encourage the external community through the existing proposal system.

We intend to increase our impact in quantum materials, focusing on magnetism and superconductivity to accelerate the knowledge transfer from fundamental to application. The variety of topics in this area, the diversity of materials, and the number of ILL scientists working in the field has resulted in something of a fragmentation of internal communication and research efforts. Closer collaboration between ILL scientists in different instrument groups would improve the efficiency and impact of their research, would raise the profile of the ILL, and would provide broader and more comprehensive support for meeting the neutron needs of the external community. The new Hub mechanism provides a framework to facilitate consolidation, taking full advantage of the experiment opportunities offered by the completion of the Endurance programme, and will reinforce and coordinate theoretical and computing support for quantum magnetism to the benefit of all.

The ILL will thus establish a Science Hub with ambitious, but achievable, objectives in a dedicated sub-field that is strongly dependent on experiments with neutrons, aiming to have a significant impact within a 3 to 5-year period. The chosen sub-field must leverage a prominent existing strength of the ILL, namely the experience and expertise of its staff. The topic must have sufficient overlap with their scientific interests to attract and inspire enthusiastic participation. A well-chosen sub-field would have significant outreach, drawing on existing collaborations and improving communication with existing networks while serving as a beacon to attract the attention of the broader community.

Much has been written about the so-called second quantum revolution[12] and its societal impact, where quantum properties are being manufactured and tailored for use in technology. Neutron techniques are particularly powerful at the earliest stages of device development in identifying and characterising quantum properties of larger samples and testing theory models in suitable materials. The focus of the Hub will therefore be on fundamental studies, investigating the quantum properties of materials to promote and speed up the development of future applications. Neutrons are needed to determine the best materials for devices, and also to show why these are the best materials.

Examples include the study of many-body quantum entanglement[13,14], in particular in quantum-spin-liquid-like materials[15,16], providing the basis for the theoretical understanding of quantum computing. Superconductivity is a continually evolving area with a key role for neutron scattering, from understanding the microscopic origins for superconductivity[17] to the push to find ever-higher temperature superconductors, which frequently require extreme pressures[18]. Quantum phase transitions have long been a popular subject[19], with neutron experiments on condensed matter having relevance to questions in particle physics and cosmology. Coupling between the structural and magnetic degrees of freedom on the atomic scale drives many physical processes but is currently poorly understood. Important examples are found in technologically important subjects such as multiferroics[20], magnetocalorics[21], and van der Waals compounds[22,23], and also in the stabilisation of exotic quantum states of matter, where the role of disorder in the atomic structure is increasingly being recognised[24]. Topological magnetism[25], which includes solitons[26], is very attractive for quantum computing and spintronics applications. Neutrons offer huge advantages in identifying and characterising materials that may host topological magnetic structures and dynamics. Very recent emergent areas include altermagnetism[27], a new type of magnetic structure with applications in spintronics, and quantum active matter[28], where theories are being developed that could link quantum physics and biological behaviour. Any of these sub-fields would serve as a suitable choice for the Hub and, once established, the Hub would provide the flexibility for coordinated and rapid support to study new materials and areas that will emerge in the coming years.

Possible expansion of in-house computation capabilities for quantum magnetism calculations, including Density Functional Theory and Molecular Dynamics, will figure prominently in the discussion and will offer opportunities to the broader quantum magnetism community.

3.3 SCIENCE HUB ON LIQUID-LIQUID PHASE SEPARATION

- We will establish a Science Hub on Liquid-Liquid Phase Separation, which will focus on problems relevant to human health and pathology.
- The Hub will consolidate internal expertise and strengthen collaborations with the Institute for Structural Biology (IBS) and the European Molecular Biology Laboratory (EMBL).

The ILL is uniquely placed among European neutron sources in having the appropriate instruments with access to all the relevant length and time scales and with the necessary resolution for the study of macromolecular dynamics. Neutron scattering and spectroscopic measurements performed by a large user community at the ILL underpin research in a diverse range of life science fields, including biophysics, food science, structural biology, hybrid nanostructures, soft matter, pharmaceutical formulation, vaccine development, and drug delivery. The ILL complements this instrument suite with expert scientific staff who work to enable users to make the best of their data. The ILL is well placed to have an impact in the rapidly growing field of Liquid-Liquid Phase Separation (LLPS). LLPS is a process where two or more liquid phases form from a homogeneous solution, typically in response to changes in temperature, concentration or other factors. In LLPS, molecules in a solution undergo self-assembly to form distinct liquid droplets, creating two coexisting liquid phases: a dense phase (the droplet) and a dilute phase (the surrounding solution). This process is driven by weak, multivalent interactions, such as hydrogen bonds, hydrophobic interactions or electrostatic forces, which are reversible and can be regulated. LLPS plays a crucial role in the formation of biomolecular condensates, which are membrane-less organelles in cells (e.g. nucleoli, stress granules, P-bodies). These condensates often concentrate specific proteins, RNA, or metabolites, allowing the compartmentalisation and regulation of cellular processes which are being shown to play important role in biology and health. These processes play prevalent physiological roles in plants, animals and bacteria. Several important cellular functions are driven by the specific local aggregation of macromolecular complexes into large functional clusters, or condensates, by LLPS[29], as demonstrated in Figure 2.

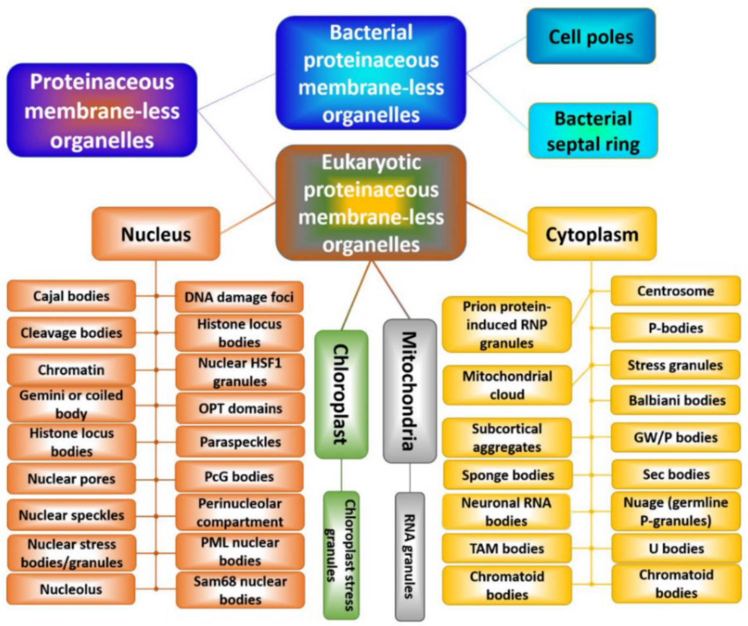

Figure 2: Multiple cellular functions are served by condensates of various bio-macromolecules in specific locations in biological cells. This figure shows an overview of examples of LLPS called "membrane-less organelles"[29].

Furthermore, there is increasing evidence that such condensates play a role in multiple pathologies, such as cancer and viral infections, neurodegenerative diseases and diseases of ageing (Figure 3). Most of the diseases result from aberrant phase separation, creating protein aggregation that disrupts the cellular function, initiates gene mutation or uncontrolled cellular division. The main strategy to prevent aberrant phase separation is to use small molecules as inhibitors.

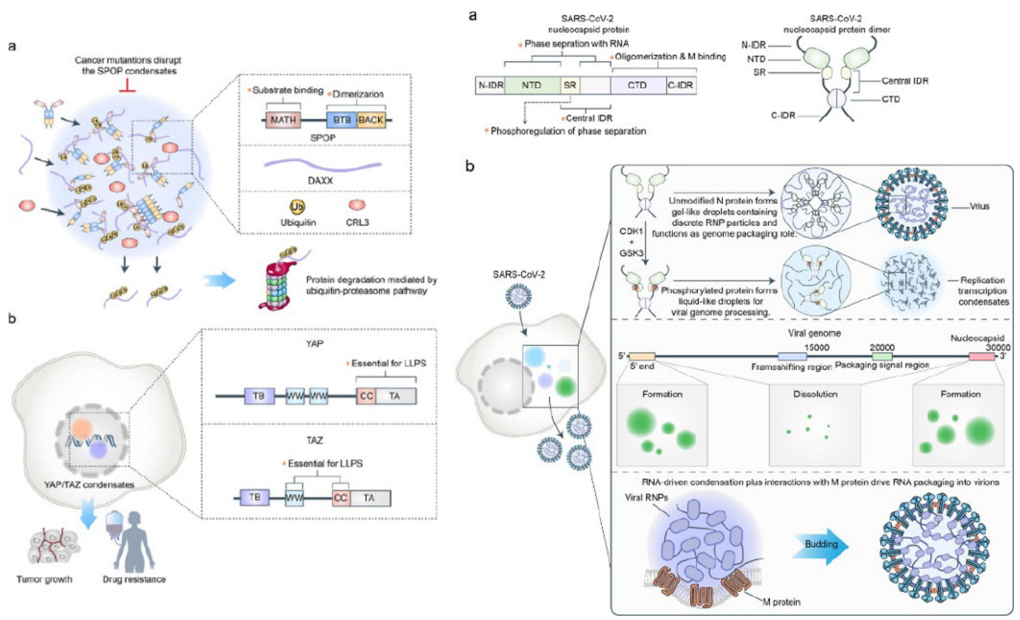

Figure 3: LLPS and condensates in cancer (left) and SARS-CoV-2 (right). The formation as well as the internal structure of the condensates depends, among other parameters, on the specific sequences and mutations of its components, and on the presence of molecules released from pathogenic particles[30].

Phase separation is also increasingly recognised as playing an important role in the structure and properties of rafts in lipid membranes, more specifically for lipid nanoparticles, which are used for drug delivery and RNA vaccines. Finally, an important class of LLPS play a role in degenerative diseases such as Alzheimer's and amyotrophic lateral sclerosis.

The study of the structure, topology and dynamics of condensates formed by LLPS is notoriously challenging for individual structural biology techniques due to their non-crystalline nature, variable morphology and poly-dispersity. The bulk of current work is focused around fluorescence microscopy methods and biophysical tools, such as light scattering and small-angle X-ray scattering. However, neutron scattering and spectroscopy have great potential to deliver new insights, and the community is beginning to take note. The neutron methods provided by ILL instrument suite cover a large range of relevant length- and time-scales involved in LLPS that are complementary to other techniques. Neutrons are sensitive to light elements, particularly hydrogen, and contrast-variation techniques exploiting the different neutron scattering probabilities of protonated and deuterated hydrogen give unequalled insight into biology-related science. The specific deuterium labelling of proteins, RNA/DNA and lipids allows the structural and dynamic properties of large condensates to be decoupled, revealing the behaviour of distinct subunits within them, which is ideal for multi-component systems. Finally, neutrons do not induce radiation damage, and biological samples can be exposed over long periods of time without impacting their structure or function, raising the possibility for *in situ* and *in vivo* studies.

We propose to develop this area by establishing a Science Hub on LLPS to consolidate internal collaboration between ILL scientists, to promote the involvement of the external scientific expertise of the Institute for Structural Biology (IBS) and the European Molecular Biology Laboratory (EMBL), and to reinforce the infrastructure support for sample preparation in biological deuteration and lipid extraction. The Hub will provide a comprehensive view of a dedicated sub-field using a combination of multiple neutron techniques and will be supported by the ILL Biology, Deuteration, Chemistry and Soft Matter support laboratories.

The societal impact of the Hub will be maximised by focusing on LLPS systems related to human health and pathology. There are many possibilities, including the interaction and condensation of different proteins with RNA in the formation of LLPS in neurodegenerative diseases like Alzheimer's[31] and amyotrophic lateral sclerosis[32], the role of protein phosphorylation in the formation of transcriptional protein-RNA condensates and its relation to disease[33], and the disruption of functional protein condensates of the protein degradation pathway by proteins displaying mutations found in cancer[34]. As for the other Science Hubs, the predominant focus and selection of objectives will be decided as part of the process of appointing the Science Hub coordinator.

Irrespective of the choice, the neutron approaches and developments within the Hub will progress with a view to versatility and applicability to a wide range of bioscience fields with similar demands. Lipid nanoparticles, which have become increasingly important as drug-delivery systems (e.g. mRNA vaccines), represent an important recent example. Their complex internal structure of RNA, proteins, lipids and sterols, and their interaction with (model) membranes, can equally be studied by neutron scattering approaches.

3.4 SCIENCE HUB ON LI-ION BATTERY RESEARCH

- We will establish a Science Hub on Lithium-ion Battery Research.
- The Hub will consolidate and expand the research efforts on battery materials, reaching out to the community.
- We will develop electrochemistry equipment and expertise, with a particular focus on *in situ* experiments.
- The Hub will build upon current efforts in collaboration with the ESRF and the CEA.

High-performance, lightweight batteries are now undeniably essential for applications ranging from the needs of a mobile communication-intense society to requirements that individual modes of land transport must reduce or eliminate emissions of CO_2, noxious gases and particles. Battery production and performance are key for competitiveness in the global economy. Challenges are focused on the performance and lifetime of Li-ion batteries, including charging speeds, Li-plating, safety and degradation. Neutron diffraction, spectroscopy and imaging can contribute to answering these challenges. Specific questions concern the formation and evolution of the solid-electrolyte interface, the diffusion mechanisms, and the characterisation of nanocomposites and polymer dynamics. There is an accelerated deployment of next-generation materials, e.g. low/no Co cathodes, Li-sulphur, Na-ion and 'generation-after-next' chemistries, e.g. K-ion and aluminium, where neutrons are a powerful probe to provide necessary knowledge. All-solid-state batteries (ASSB) are currently a very active field[35], thanks to the promise in terms of safety and higher energy density, and neutrons can be used to probe their fundamental mechanical behaviour.

The strengths of neutron techniques in battery research lie in their unique sensitivity to light elements (Li, Na, H_2), their high penetration that allows straightforward *in operando* experiments, and the ability to differentiate between atoms with similar mass, such as Ni, Co and Mn, which are crucial components of "LMNO" cathode materials. These latter materials are also magnetic, which may play a part in their electrochemical behaviour, and neutrons are particularly suited for the study of magnetic structures and dynamics.

Neutron studies *in situ* are particularly powerful, both using diffraction and, thanks to the high neutron attenuation of lithium, imaging techniques[36,37]. Figure 4 shows an intuitive example of the power of *in situ* neutron powder diffraction, revealing that non-stoichiometric Li-manganate cathodes show less capacity fading because a stoichiometric compound goes through two reconstructive phase transitions during a charge-and-discharge cycle while a non-stoichiometric compound simply and smoothly changes lattice parameters[38]. SANS and spectroscopy techniques can provide a unique insight into diffusion mechanisms for lithium, and additionally for sodium-ion materials.

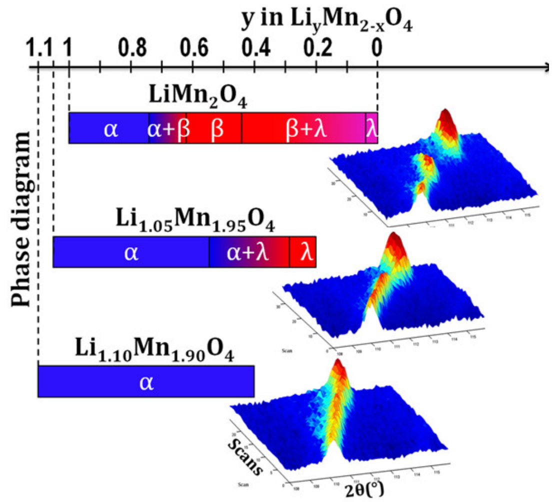

Figure 4: Phase transitions in spinel electrode materials subject to an electrical charge-and-discharge cycle. Reprinted with permission from [38]. © 2014, American Chemical Society.

Battery research has been a hot topic for a number of years and other neutron facilities (e.g. PSI, MLZ) have made strategic investments to give themselves a competitive edge. The ILL has recently made a considerable effort to catch up and is now involved in multiple different research programmes, attracting PhDs and post-docs and investing in infrastructure and lab space. The success of these efforts is evident in the high demand for beam time, which we sometimes struggle to satisfy, but we are confident that we can further improve our impact in the field to become a clear leader amongst neutron scattering centres. Particular efforts will be made to improve capabilities and expertise in electrochemistry, with special attention paid to handling sensitive samples and to *in situ* sample environment, to consolidate and bolster internal expertise to serve the community, and to attract and retain external groups. We intend to create a Science Hub to serve these purposes. The ILL may be able to learn from an existing initiative currently running at ESRF in collaboration with CEA Grenoble[39], and will work to build cross-campus support including connections to the GIANT environment (Minatec, etc.).

The Hub will establish and maintain an electrochemistry laboratory as a support infrastructure, potentially in collaboration with ESRF. The laboratory will build upon currently-available equipment, including a dedicated electrochemistry glove box close to the diffraction instruments D20 and D2B, a multi-channel charging cycling device and, with examples shown in Figure 5, several battery cells for *in operando* neutron diffraction and imaging experiments[40,41]. Further equipment and consumables will be added, such as neutron-compatible *in situ* battery cells, charging stations, deuterated electrolytes and dedicated glove boxes, both in the guide halls and outside the radiation-controlled areas. The laboratory will be established in close collaboration with external groups, with the aim of allowing them to prepare samples properly and test equipment ahead of experiments and to perform follow-up measurements post-neutron beam time.

The Hub will require human resources. Technical assistance will be required to manage the laboratory, and to design and build other suitable battery cells for *in operando* experiments. ILL scientists will be encouraged to participate and expand the expertise, with clear experimental needs requiring diffraction, strain scanning, SANS, imaging, QENS and neutron spin echo instrumentation. The Hub will be supported by students and post-docs, and will host visiting students and scientists. It will serve as a convenient access entry-point for external users working on batteries, allowing them to discuss and plan neutron scattering experiments, meet experienced staff, and have a fruitful exchange of ideas and solutions.

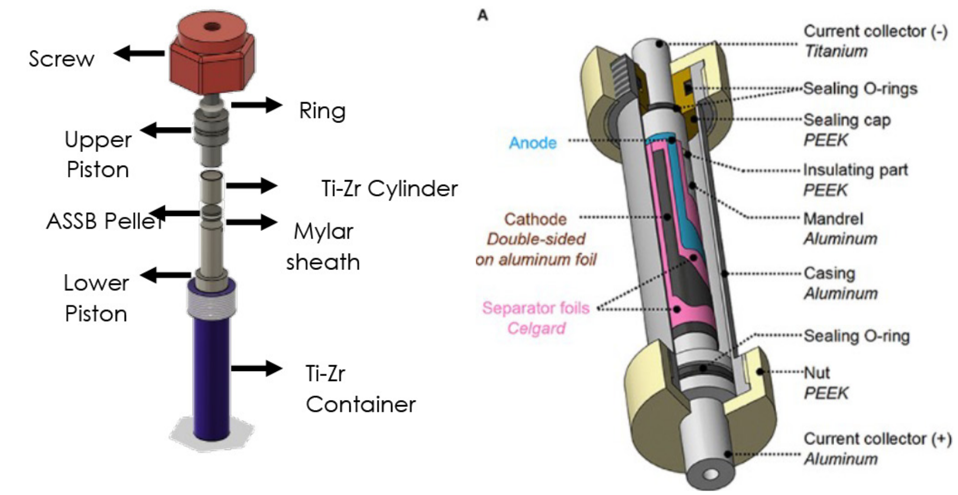

Figure 5: (left) The ILLBAT#5 pressure-monitored electrochemical cell for *in operando* experiments (right) A cylindrical cell, double-coated electrode with 5 g of sample, similar to commercial batteries, encased in TiZr[41].

3.5 SCIENCE HUB ON ADVANCED MANUFACTURING

- We will establish a Science Hub on Advanced Manufacturing
- The Hub will consolidate and coordinate industrial research at the ILL, with a focus on additive manufacturing.
- The primary experimental techniques will be imaging and strain scanning.
- Software to quantify stresses and analyse imaging data will be developed.
- The Hub will strengthen connections with ESRF efforts dedicated to additive manufacturing.

The complexity of fabrication technologies and new materials for engineering components has increased substantially, particularly in the last decade. Innovative solutions are necessary to address modern industrial needs while reducing energy consumption and waste, and all require verification of their quality and behaviour, including under operating conditions.

One of the most exciting recent developments has been in additive manufacturing, or 3D printing of advanced materials. Additive manufacturing has become a transformative technology in industrial applications due to its capacity for precise, layer-by-layer fabrication of complex geometries, enabling the production of custom components with intricate internal structures and minimising material wastage. It is particularly advantageous in fields such as aerospace and biomedical engineering, where lightweight, high-strength parts and patient-specific implants are essential. The technology enhances manufacturing efficiency by enabling rapid prototyping and allowing on-demand production, and supports the development of advanced materials, including metal alloys and composite materials.

New materials and processes bring with them new uncertainties, for example related to porosity, as well as inhomogeneous and/or metastable microstructures due to complex 3D thermal gradients coupled with new fabrication parameters. This hinders the understanding of their behaviour under operando conditions and ultimately prevents their final approval as new engineering components in terms of their safety and durability (level TRL 9 (System Proven and Ready for Full Commercial Deployment) in the EU). There is a particular opportunity for the ILL to engage in a dedicated industrial research collaboration to cover steps TRL 4 (Lab Testing/Validation of Alpha Prototype Component/Process) to TRL-6 (Prototype System Verified) in the EU classification process for new engineering components.

Thanks to their deep penetration and their unique interaction with matter, neutron methods are an excellent probe for industrial applications. Two high-impact neutron techniques for this type of research are imaging and strain scanning.

Neutron diffraction is well-known and recognised in the academic community for internal strain-stress assessment of polycrystalline materials (ISO 21432:2019 Non-destructive testing (NDT) — Standard test method for determining residual stresses by neutron diffraction[42,43,44]). It is considered validated in the laboratory environment and may therefore be classified as TRL 4. The neutron diffraction method is the only NDT method that provides a full strain-stress tensor analysis with particularly high lateral resolution, probing from near-surface (~100 μm) into the bulk (~10 cm). The ILL operates SALSA, a state-of-the-art strain scanner with the highest flux and spatial resolution at sample position world-wide, which is used extensively for industrial research. In recent years and in order to meet industrial demand for access to highly sensitive and non-destructive characterisation techniques, the ILL has been involved in two EU projects as a partner. The Brightness2[45,46] project (2029-2021) defined common calibrants and standard operation procedures for the neutron strain community (ISIS, ILL, FRMII, NECSA, future ESS and PSI), resulting in the creation of the Neutron Quality Label® trademark. The EASI-STRESS project (2021-2024) validated the use of combined X-ray, synchrotron and neutron diffraction for industrial applications and case studies, moving neutron diffraction residual stress techniques towards TRL 6-7. More recently, neutron strain diffractometry was used to study stress relaxation during post-processing treatments such as heat treatment or hot isostatic pressing, which are commonly used to reduce residual stresses and enhance the mechanical properties of parts made using additive manufacturing, as shown in Figure 6.

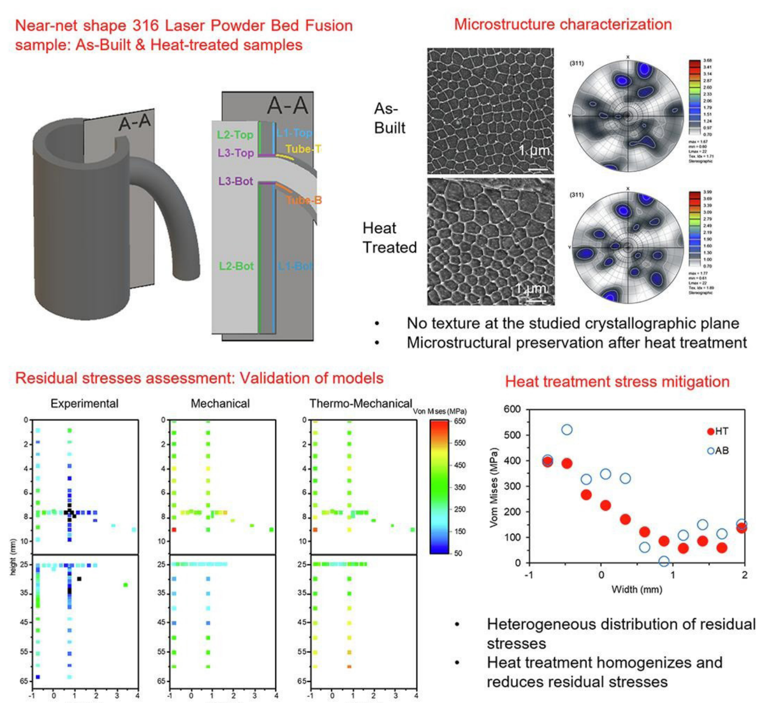

Figure 6: Graphical abstract from[47], where a 316L laser powder bed fusion sample is tested, including SEM, residual stress assessment as a function of the position and effect of heat treatment stress mitigation strategies.

Neutron imaging has emerged as a versatile and powerful experimental technique, particularly for industrial research. The ILL now operates NeXT, a cold neutron imaging instrument with the highest flux and spatio-temporal resolution worldwide. The white beam methods employed by NeXT are able to image fabrication microdefects and their spatial distribution with a resolution of a few microns[48]. The non-destructive, full-geometry nature of imaging allows nearly arbitrarily sized and shaped samples to be studied, and the high flux of NeXT allows real-time measurements to study devices *in operando* and defect formation during fabrication. There is great demand for the ILL to increase its capacity and capabilities with this popular and rapidly expanding technique, which we will address as an important part of the Science Strategy (section 4.1). Applications in industrial research will be an essential element for the development of additional imaging capabilities.

Given the scientific and industrial potential that neutrons can offer, a Science Hub on Advanced Manufacturing is proposed. The complementarity of information between imaging and strain scanning is evident, and the Hub will strive to take full advantage of this by consolidating experimental programmes across these multiple techniques, in close coordination with industrial outreach. The Hub will have a focus on additive manufacturing, where the ILL is already active[49]. Reproducing realistic procedures is crucial to be representative of industrial needs. Particular efforts will therefore be made to create sample environments for *in situ* and *in operando* testing that are adaptable across multiple instruments and facilities. The high flux, high lateral and spatial resolution, and flexibility in sample space and environment offered by both NeXT and SALSA, combined with the continuous acquisition of neutron signal[50], will allow new experiments to be carried out, such as *in situ* additive manufacturing printing and stroboscopic fatigue tests, and will offer new possibilities for exploring the strain-stress formation, kinematics and evolution.

The Hub will also coordinate computing efforts to model and analyse data. Internal strain-stress analysis in advanced manufacturing relies on predictions from analytical and finite element modelling of 3D residual strain and stress distributions. The modelling methods cannot fully account for all real-life conditions. Conversely, neutron measurement techniques each have their own sources of uncertainty. An effective approach would thus use numerical modelling to predict and quantify residual stresses and then to validate them through *in situ* and non-destructive neutron measurements. Artificial intelligence (AI) will also be an important computational tool. AI methods are transforming the analysis of real-space data from fields such as Cryo-EM[51] and may be adapted to interpret results from neutron imaging experiments. Furthermore, AI is playing an increasing role in residual stress analysis, and the precision offered by neutron techniques has great potential in training AI algorithms[52].

The ESRF has similarly recognised the importance of additive manufacturing, and there is currently extensive activity focused on *in operando* experiments using its imaging and strain beamlines[53]. The Hub will strengthen the existing link with this ESRF powerhouse to take advantage of the unique capabilities and expertise of their instruments and scientists.

3.6 SHOWCASE EXPERIMENT ON SUPERCONDUCTING WIRES

- We will establish a Showcase Experiment to address the challenges involved in the scaling-up of the production of high- and low-temperature superconducting wires.
- Measurements under *in operando* conditions (e.g. at 20 K and in a 20 Tesla field) and the effects of radiation damage are of particular interest.
- Imaging, strain scanning and SANS are potential experimental techniques.

Beyond the case for continuing fundamental studies in quantum materials, neutrons have potential to address some of the challenges facing the exploitation of quantum properties in application-ready devices. Particular challenges arise due to the need for mass production, scalability and cost-effectiveness, which ultimately may limit device applicability and therefore societal impact. Superconducting (SC) wire manufacturing is a prominent example of an area facing such demands while simultaneously presenting opportunities for neutron research to contribute to its success. We therefore propose to develop and perform a Showcase Experiment to demonstrate the potential for neutron scattering in advancing industrial-scale SC wire technology.

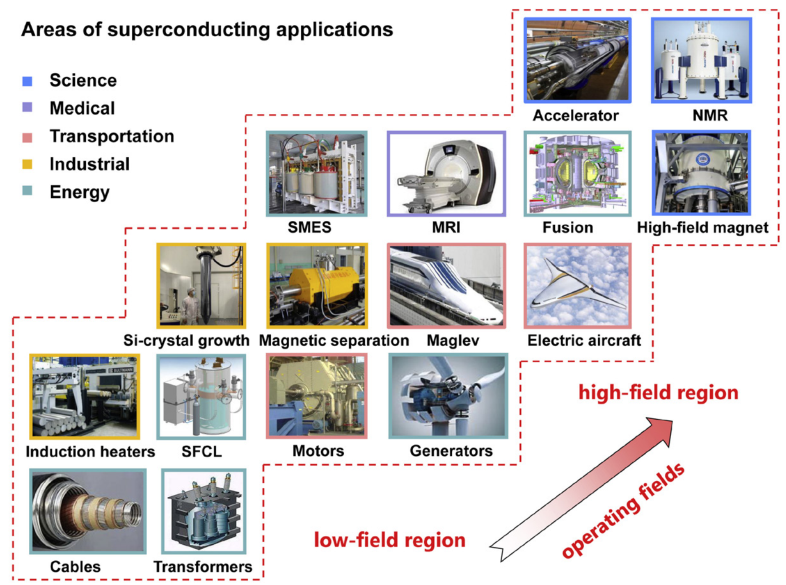

Figure 7: Examples of applications in different societal areas for magnets based on superconducting wire technology. Reproduced from[55].

A team of ILL staff will liaise closely with relevant external partners to design a proof of concept tackling real needs. The experiment should make the best use of currently available equipment at the ILL to be achievable within a 2-year period.

Superconducting wires already have a huge societal impact due to their use in magnet technologies employed in the medical, clinical, mobility and energy sectors (Figure 7)[54,55]. They form the central component in magnetic resonance imaging[56] and hold the promise of bringing nuclear fusion reactors from the laboratory to the electrical grid[57]. In 2023, the Grenoble-based company Renaissance Fusion received a € 10 million grant from the "France2030" programme to commercialise fusion reactors by 2030s[58]. With ITER, a major international construction effort is underway in southern France to construct a full-scale Tokamak device to prove the feasibility of fusion as a carbon-free energy source[59].

Today's industrial SC wire components are based on low-temperature superconducting (LTS) wires, which require expensive liquid helium cooling and cryogenic designs to operate at their critical temperature. High-temperature superconducting wire (HTS) may alleviate many of these cost constraints, promising usability even above the boiling point of liquid nitrogen.

Both categories of materials face urgent challenges due to the need to produce large quantities with reliable performance. Quality control becomes a leading issue in the scalability of SC wire manufacturing since the critical current above which the material becomes a normal conductor is determined by the weakest part of the wire. HTS materials are highly sensitive to the elemental stoichiometry and grain structure, allowing only small variations before their performance deteriorates. Furthermore, current wire technologies are based on SC tape wrapped around or embedded in copper cores, leading to potential micro cracks and critical deformations, which limit the critical current. Homogeneous SC properties and quality must therefore be ensured tape-by-tape on several hundreds of km of wire, which is typically performed in reel-to-reel type experiments.

Significant challenges relating to device operation also need to be considered. For example, the self-field screening effect limits the maximum field and the rate at which a SC wire coil can be operated. Training effects and deformations during operation further affect the performance of SC wire magnets. The construction of fusion reactors comes with the key problem of fast neutron radiation damage to the SC windings around the plasma chamber[60]. After an initial increase in performance, the critical current drastically decreases above a fluence of the order of $10^{18}/cm^2$, but more data is needed to fully understand this process. The effect of thermal neutron irradiation is not limited to HTS wires, but is important to consider in LTS components as well as the complex stack of materials surrounding the SC.

The Showcase Experiment on Superconducting Wires aims to establish the feasibility of neutron scattering to address some of the challenges faced in SC wire technology. A key parameter for SC wires is the current density and penetration depth, which can be revealed by small-angle neutron scattering. Neutron imaging experiments may focus on large-scale uniformity and fault detection in certain sections of the device. Strain scanning under *in operando* conditions may be envisaged to determine the strain distribution arising from magnetic and thermal strain. Concerning the effect of neutron irradiation, the ILL may explore possibilities to perform thermal neutron irradiation on different materials in controlled conditions. Possible experiments will be considered for both HTS and LTS wires. Ideally, the experiment would take place under *in operando* conditions. The ILL has access to low-temperature and high-field equipment that may be appropriate, for example the 17 Tesla Birmingham cryo-magnet for SANS experiments.

The final form of the Showcase Experiment will be designed by a team at the ILL. However, appropriate involvement of external research institutes and industrial partners will be the key to its success. The team developing the Showcase Experiment at the ILL will need to partner with and focus on the needs of these external parties to keep the experiments as close to real world conditions as necessary.

3.7 SHOWCASE EXPERIMENT ON CELL STRUCTURE WITH HIGH-RESOLUTION BIO-IMAGING

- We will establish a Showcase Experiment on Cell Structure measured using High-Resolution Bio-imaging.
- The possibilities of neutron imaging with 4 μm resolution for bio-imaging experiments will be explored.
- The experiment will require close consultation with EPN partners on our shared campus: EMBL, IBS and ESRF.

Neutron imaging has been applied to a multitude of biological systems to probe structural features at the level of tissues and organs, as well as for several medical applications[61]. Figure 8 shows an example of neutron tomography being used to study the time-dependent water uptake by maize roots, monitored with a time resolution of a few seconds and a spatial resolution of 100-200 μm.

The recent advances in high-resolution (≤ 4 μm) imaging using neutrons[63] are potentially extremely exciting for the life science community. Neutron imaging has the potential to provide unique information that is complementary to the current state-of-the-art in the imaging of cells, tissues, and whole organisms, with μm resolution using X-rays, electrons and light.

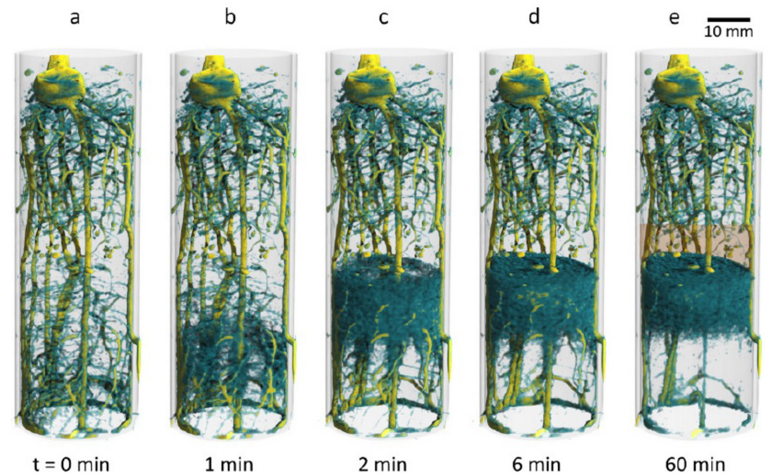

Figure 8: Water uptake in maize roots with fast neutron tomography[62].

The unique benefits of neutron imaging are due to their cross-section (penetration and contrast properties) and the possibility of altering transmissions by deuterium labelling of macromolecules and H_2O/D_2O exchange. The high visibility of fluids and hydrogen-rich phases to neutron imaging is of crucial interest in biological tissues. Furthermore, due to the damage-free nature of neutron imaging, there is also the exciting possibility of examining living processes in real time. Improved spatial resolution would be desirable and, if it could be achieved, a 1 μm resolution would be particularly exciting, as this would allow eukaryotic cells (10-50 μm) to be mapped efficiently at a subcellular and organelle length scales. However, there are possibilities even with the present resolution. For example, Figure 9 shows a recent demonstration at EMBL-Hamburg of high-throughput μm-scale imaging of whole organisms (on the mm scale) that has created tremendous excitement in the biology and ecology communities[64]. These tomographic experiments map each cell and were performed on fixed samples, allowing population level changes to be followed (for example, parasitic infection processes, or mutations and morphological alterations due to environmental changes). The experiments show that previously inaccessible questions can now be addressed. Performing similar experiments, in a damage-free manner allowing for the study of living organisms, would be a potential game-changer for the community, opening an entire new life science user community at the ILL and mapping onto the research agenda ("From Molecules to Ecosystems"[65]) of campus partner EMBL.

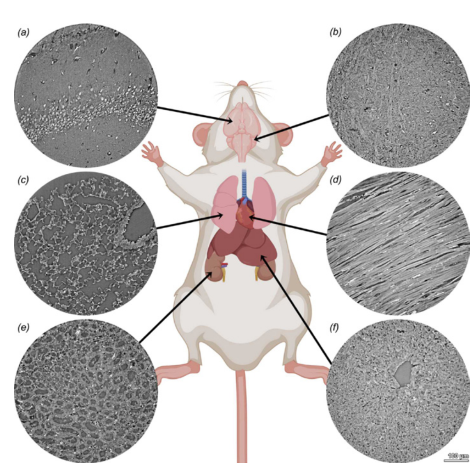

Figure 9: Application of X-ray tomography for murine tissue histology[64]. © Biorender

We will perform a Showcase Experiment exploring the capabilising of neutron imaging for the study of biological systems. The experiment must be carefully chosen, capitalizing on the complementarity of neutrons with respect to existing optical imaging methods and tomography using X-rays and Cryo-EM. The absence of radiation damage, the capacity to penetrate bulk matter (~mm), the sensitivity to isotope labelling (H_2O/D_2O exchange and macromolecular deuteration) represent unique strengths of neutron imaging, but also a framework and guidance for the choice of biological systems to be studied. There is a need to monitor the influence of infection, pathology, and environmental stress[65] on the characteristic structural features in a broad variety of conceivable systems covering length scales from whole organisms to tissue structure to morphological features of eukaryotic cells.

The experiment must be achievable with current instrumental resolution (~ 4 μm), and the choice of the subject will require close consultation with our partners within the Partnership for Structural Biology (PSB: IBS, ESRF, and EMBL). Input from the EMBL will be particularly important, following their recent imaging experiments.

3.8 SHOWCASE EXPERIMENT ON WATER MEMBRANES FOR A SUSTAINABLE FUTURE

- We will establish a Showcase Experiment to explore the possibilities of using neutron techniques to study membranes used for water treatment.
- SANS, reflectometry, QENS and imaging are potential techniques.

Issues involving the environment and sustainability are currently recognised as having an enormous impact on society. Human activity has consequences on a global scale, from pollution to climate change. Establishing actions to change human behaviour to minimise the environmental footprint has been recognised by the EU and forms a development goal of the UN. Access to fresh-water is included as a separate pillar of the United Nations Sustainable Development Goals[66]. Fresh water is needed for drinking water and agriculture, and is critical for sanitation, industry, and power generation. According to the UN report, about 30% of the world's population live in so-called "water-stressed" countries, where the majority of people lack safely managed drinking water. These countries are mainly in the developing world but, when projecting into the intermediate future (~50 years from now), many developed countries will also be facing fresh water scarcity due to climate change, contamination and a growing population[67]. As only ~1% of the Earth's water is considered to be "fresh", desalination has increased fivefold in the last twenty years, and some regions are extremely dependent on it. Desalination plants supply 70% of drinking water in Saudi Arabia, 90% in Kuwait, and 42% in the UAE.

Although many methods are currently used for water filtration and desalination nowadays, membrane materials and processes are considered state-of-the-art and seminal for future technology thanks to their advantages, which includes high separation efficiency, easy operation, low energy consumption and environmentally-friendly properties[68]. Initially, only polymer-based membranes were used for water filtration and desalination[69], but more recently very thin metal-organic framework materials (MOFs) in quasi 2D arrangement (nm-thickness) are showing the best performances[70]. Sandwiched between MXene layers, these 2D MOF/MXenes composite membranes show both high performance and long-lived stability, essential for final applications[71]. These types of membrane approaches can also be applied to control salinity gradients between river water and seawater in estuaries for osmotic energy generation (blue energy).[72]

Neutrons have the potential to make a real impact in this field, particularly due to their sensitivity to hydrogen and the ability to apply contrast variation methods via deuteration. The high penetration power of neutrons combined with their light element sensitivity also facilitate *in situ* and *in operando* studies. As the ILL currently does not have a strong presence in this rapidly growing area, in particular where the most recent types of membrane materials are concerned, we would consider it to be premature to consider building a Science Hub capable of providing a significant results within a nominal 3/5-year period.

However, we see a strong opportunity to show the potential for neutron techniques and to attract an important community with a Showcase Experiment on state-of-the-art membranes for water treatment.

The unique combination of several world-leading neutron-based instruments available at the ILL offers multiple possibilities, including the study of single-membrane layers by neutron reflectometry to extract the time-resolved distribution of single-molecules in or next to the membrane[69], experiments on multilayer assemblies investigated by quasi-elastic neutron scattering to extract information on the single molecule dynamics in highly-confined geometries inside the membrane[73], and using neutron imaging to extract time-resolved macroscopic concentration gradients across the membrane[74]. The ability to perform of these as in operando experiments will be carefully considered to provide higher relevance and impact.

One potential Showcase Experiment could be to extend the polymer-based membrane work for desalination (and blue energy) performed atthe ILL by groups from Imperial College London. Their experiments on novel 2D MOF/MXene composite membranes used reflectometry to resolve the water distribution[69] and spectroscopy to study the confined water dynamics[73]. The experiment would draw on a long-standing collaboration between these groups and several ILL scientists, but would depend on the groups' ability to master the fabrication and characterisation of these materials.

A second possibility in this field concerns the study of novel membranes for the filtration of emerging pollutants in our drinking water, focusing on the environmental impact of per- and polyfluoroalkyl substances (PFAS). PFAS are an emerging pollutant in our ground water due to the extensive use of fluoro-based surfactants in various applications[75]. The chemical nature of these molecules in water involves the formation of micelles and aggregates, which are readily studied using neutron techniques such as SANS, reflectivity, and QENS. ILL scientists already have a collaboration with groups from Uppsala University in Sweden[76] which could be a basis for a Showcase Experiment using reflectivity to determine the PFAS concentration inside or next to a novel membranes.

4 Common implementation mechanisms

The ILL has a number of activities that cut across scientific areas and can be expanded or improved to maximise their overall scientific impact and relevance. These activities would benefit all the scientific endeavours of the ILL, across Colleges, Science Hubs and Showcase Experiments, and were prioritised in the conclusions of the Science Strategy Working Group. This section describes these activities, and the intended actions within the Science Strategy.

4.1 NEUTRON IMAGING

- The popularity of and demand for neutron radiography and tomography are rapidly increasing. We recognise that the ILL must boost its capacity and capabilities in these techniques.
- A new dedicated thermal neutron imaging station (ThRILL) and a portable cold neutron tomography station (PorTo) will be built.

Modern imaging techniques are able to provide quantitative 3D maps of the internal structure of samples with complex and heterogeneous microstructures. They are often combined with complex sample environments reproducing real conditions. Very importantly, given the non-destructiveness of the techniques, processes can be investigated *in situ* and *in operando* to study the time evolution of a material. These capabilities are at the heart of a veritable revolution in a growing number of fields, such as energy, sustainability and health technologies.

Demand for imaging and tomography is growing rapidly, and is proving to have a crucial role in science for society. This is clearly visible in the market for commercial X-ray tomographs, numbering in the several tens of thousands, and at synchrotron radiation facilities, which typically have a large (and increasing) number of imaging stations. It is also clearly visible in the demand for appropriate neutron instrumentation, with heavy oversubscription for experiments on NeXT, currently the only neutron imaging instrument at the ILL. Neutron radiography and tomography were highlighted as extremely important experimental techniques by the Science Strategy Working Group, offering new and exciting opportunities in current and emerging science areas, and this is evident in the expected demand from the proposed Science Hubs and Showcase Experiments. The Working Group gave a strong recommendation to increase capacity and capability with these techniques.

Neutrons are strongly complementary to X-rays. The unique nature of neutron radiation gives high sensitivity to light elements, isotope sensitivity (in particular the possibility of performing isotopic labelling with deuterium), significant penetration depth and sensitivity to magnetism and magnetic fields. Combined neutron and X-ray imaging measurements are particularly powerful in unravelling coupled processes, such as the electro-chemo-mechanical processes driving battery degradation[77] or the thermo-hydro-mechanical processes driving the aging of construction materials[78]. The complementary information provided by the two forms of radiation help unravel these complex interactions.

Neutron imaging can cover length scales spanning multiple orders of magnitude from metres (for example cultural artefacts[79], and real-scale industrial components) to microns (for example dendrite growths in batteries[80] or electrolyser cells[81]). More advanced imaging techniques, for example neutron grating interferometry, giving a SANS-like contrast[82], and dark-field imaging methods[83], can give access to shorter length scales. Neutron imaging generally has lower spatial resolutions than X-ray imaging but, if combined with a simultaneous high-resolution X-ray imaging at the neutron instruments, as well as new AI-based algorithms, and ongoing detector developments, higher resolution using neutron imaging can be achieved. Neutron imaging can be used to follow time-dependent processes from the very slow processes (e.g., corrosion[84]) to the relatively fast ones (e.g., fluid uptake in plant root systems[85]). The breadth of accessible length- and time scales makes neutron imaging a truly versatile technique for a broad range of scientific studies with societal impact, as highlighted in Figure 10.

Further technical developments and options extend this versatility. Bragg-edge imaging is an emerging technique, used to extract volumetric 3D maps of the strain across bulk samples in a 2D projection (thickness averaged) for a given lattice family[86], and provides information which is complementary to strain scanning. Polarized neutron imaging can be used to study the spatio-temporal distribution of even sub-percent fractions of ferromagnetic phases that are present in stainless steel and copper alloy composites, which can in turn be associated with the local temperature fluctuations during processing.

Presented with the existing demand and the potential for imaging techniques, the ILL finds itself severely capacity-limited with only one dedicated high-performance imaging instrument: NeXT. The lack of capacity has broader ramifications, especially when considering today's challenging European neutron eco-system. The cold neutron instrument NeXT is world-class with high resolution and a broad portfolio of contrast options available, but the high oversubscription severely affects the number of applications that can be explored and the time that can be allotted to each of them.

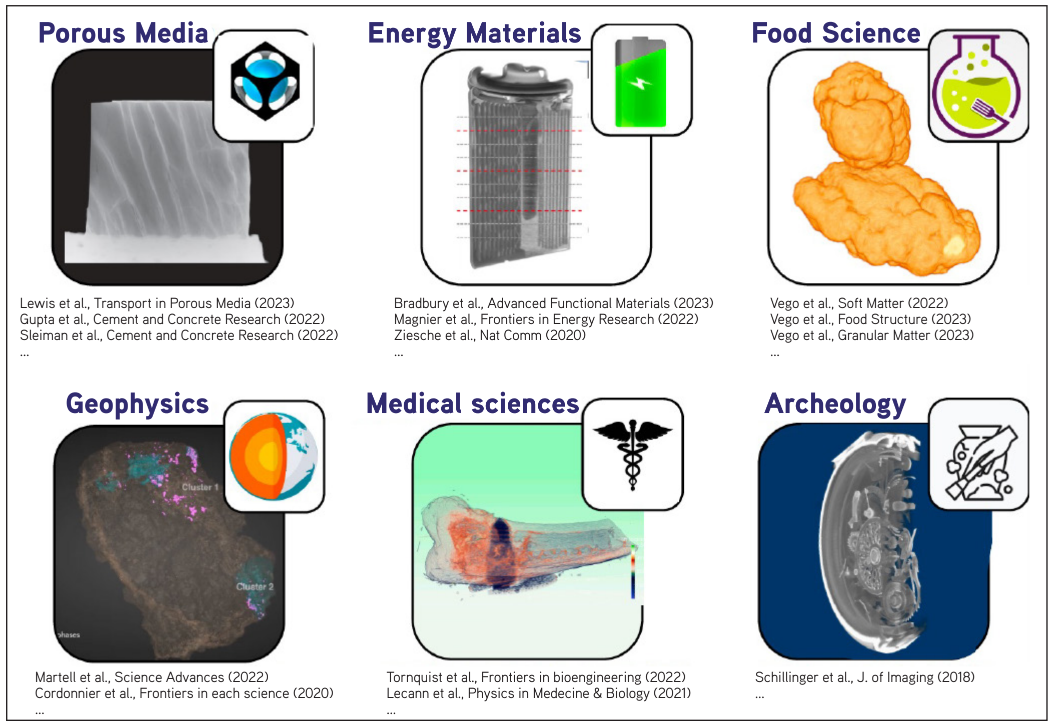

Figure 10: Fields relevant for the application of neutron imaging.

We intend to implement more capacity for neutron imaging, possibly combined with high-resolution X-ray imaging. The implementation must be achievable on a short time scale. Two options are proposed to complement the cold neutron instrument NeXT: the thermal neutron imaging instrument ThRILL and the cold neutron portable tomograph PorTo.

We are currently studying the feasibility of building ThRILL (Thermal Radiography at ILL), a thermal neutron imaging instrument to be installed on a beam port next to the ILL reactor. The cold neutron spectrum of NeXT is key to enabling its world-record spatial resolution, but can be a shortcoming when imaging real industrial components. The higher penetration power of thermal neutrons allows significantly thicker samples to be studied, and therefore opens opportunities for more realistic conditions and industrial applications. ThRILL will benefit from a world-leading high flux (two to three times that of NeXT) and will have a large field of view, allowing it to be tailored for high-speed operando and *in situ* tests on real-scale, representative samples. Real-size fuel cells, commercial batteries, engineering materials and components will be tested in realistic as well as in extreme conditions. ThRILL will also expand the portfolio of imaging options, allowing diffraction-based and short-wavelength interferometry imaging.

To expand the capacity for high spatial resolution imaging, important for dendrite growth in batteries, carbon-neutral cement and CO_2 electrolysis, and to relieve the overload on NeXT, we are currently building PorTo, a Portable Tomograph that can be rapidly installed at the end of a guide. For example, PorTo will fit in the existing PF1B instrument, where it

could be straightforwardly installed in alternation with the ongoing nuclear and particle physics programme. PorTo will be designed with a pencil beam and for a cold spectrum, ideal for high resolution. The design will offer the highest synergy with the other imaging activities at the ILL, with NeXT focusing on high throughput, ThRILL focusing on thermal neutron imaging, and PorTo focusing on very high resolution with correspondingly long experiment durations. The addition next year of the MoTo imaging station for measurements such as Bragg-edge and dark-field imaging as part of the NeXT project will further increase the supply of imaging capacity at the ILL.

4.2 APPLIED SCIENCE INSTRUMENT GROUP

- A new instrument group for Applied Science will be created consisting of the expanded suite of imaging instruments, together with the instruments for strain scanning and irradiation, and including dedicated resources for enhanced industrial collaboration.

The expansion of imaging capabilities within the ILL leads us to create a new organisational structure within the Science Division: A new instrument group for Applied Science, which will include the imaging instruments NeXT, MoTo, PorTo and ThRILL, as well as the SALSA strain scanning instrument and the TENIS irradiation station. The techniques covered by these instruments have much in common in terms of the science they address, which is largely focused on problems with real-world applications and with direct links to immediate societal benefits.

The new instrument group will capitalise on the potential synergies between imaging, strain scanning and irradiation by promoting the development of hybrid techniques, such as diffraction-based imaging, as well as prompt-gamma activation analysis and imaging (PGAA and PGAI) to perform quantitative chemical analysis in 2D or 3D, and by pooling common sample environments, particularly for *in situ* and in operando measurements and for large-volume samples, and sharing expertise on data processing, analysis and interpretation.

The group will benefit from and enhance the increasingly important relationship between neutron scattering and industry as companies seek more efficient and sustainable methods to develop and manufacture materials, ensure quality control and optimise manufacturing processes. Stress-strain mapping and 3D imaging have the potential to become central to the development of high-quality metals and polymers used in additive manufacturing, lithium-ion batteries and nuclear materials.

We will develop new and closer types of industrial collaborations with the instruments in the group, involving mutual commitments such as shared personnel and equipment. These collaborations will be facilitated by the inclusion of the existing Industrial Liaison Unit into the new group, whose focus on supporting the instruments in the group will be complemented by a mandate to maintain the existing level of industry access to the techniques available in the other instrument groups.

Industry liaison at the ILL is often closely associated with the proprietary access route: the sale of beam time for which industry partners pay full cost for measurements with no requirement to publish, and which currently accounts for a small fraction (~1%) of overall beam time. Increases in the sale of beam time to industry could be used to augment the resources available for industry liaison.

The new instrument group will complement the existing four instrument groups (Large-Scale Structures, Diffraction, Spectroscopy, Nuclear & Particle Physics) with an emphasis on applied sciences and will benefit from the recruitment of a group leader with specific scientific and technical expertise in this area. The new group leader will have the mandate and resources to support a strengthened emphasis on collaboration with industry, primarily with the instruments in the group, but also in support of industry involvement across all ILL instruments.

4.3 DATA SCIENCE

- We will consolidate the data reduction software suite.
- We will broaden the implementation of real-time data reduction to improve experiment planning and execution.
- We will establish an integrated platform for data analysis, interpretation and simulation.
- The improved data reduction and analysis pipelines will be combined with AI and ML tools for improved performance.

A vision and strategy are presented for improving the service to users in terms of experiment steering, data reduction and data analysis. The goal is to increase the scientific impact of the institute, which – following completion of the Endurance programme – will focus on the pipeline of transforming experimental results into publications. The objective of the data science strategy is to increase both the number and quality of scientific papers resulting from an experiment performed at the ILL and to broaden our user base towards non-expert users, essentially by making better use of the beam time. This will be done by developing and implementing targeted high-quality software.

The chain leading from scientific idea to publication comprises three closely interconnected components. We will invest in each of these components, with the aim of matching the software/data service to the level of technical performance of the ILL instrument suite following the completion of the Endurance programme:

- Data Collection is concerned with how the scientific data are collected and thus the way the experiments are performed by the experimental team, as well as how the data are stored. We will develop Augmented Experiment Steering to assist experimentalists to prepare and perform their experiments, use their beam time with maximum efficiency and make full use of modern software tools.

- Data Reduction transforms the raw data into neutron observables after proper correction and transformation (space, time, wave vector, energy, etc.). This component is a central and essential prerequisite for the others.

- Data Analysis covers the know-how and numerical tools necessary to understand the experimental neutron observable, including specialised fitting software and/or simulation packages. We will develop an Integrated Platform for Analysing Data to modernise analysis packages, integrate sophisticated computational packages for Density Functional Theory and Molecular Dynamics, and improve accessibility for non-specialists.

We will investigate the use of Artificial Intelligence (AI) in all these areas, focusing on harnessing the potential of the latest AI developments wherever possible

While the scope of the data science project is potentially very ambitious, the description outlined below is intended as a basis for incremental development and implementation according to the existing status of the given component and the availability of funding, driven by priorities established from the user programme and the Science Hubs.

4.3.1 DATA REDUCTION

Data reduction involves the correction of raw data from instrument-dependent artefacts and the conversion from instrument-dependent units, such as counts, scattering angles and time-of-flight, to sample-dependent units, such as momentum and energy. It is a prerequisite for all the other steps in the publication pipeline and therefore has the highest priority.

A wide range of software is developed and maintained at the ILL to reduce the raw data produced by the ILL instruments: *Int3D* for single crystal diffraction, *Mantid* for TOF and spin echo spectroscopy, SANS, reflectometry and powder diffraction, *Takin* for 3-axis spectroscopy, *Esmeralda* for Quasi-Laue diffraction, and *Grasp* for SANS (covering both powder and anisotropic scattering).

We will consolidate the foundations, namely by maintaining and developing the existing software suite, avoiding single points of failure (e.g. by collaborative software development), continuously providing documentation, and by testing and developing API, Jupyter Notebook and other scriptable interfaces.

We will extend the range of data reduction on offer to cover the specific cases of imaging and tomography, which are of strategic importance for the ILL. The current solution for data acquisition and reduction in neutron imaging relies on a proprietary commercial software which does not offer the flexibility to cover the full range of available experimental setups and corresponding data analysis techniques. The need for an efficient, modular open-source package for imaging data is common to many large-scale facilities (both for neutrons and X-rays) and its development will be performed within a collaborative framework, allowing the control of data acquisition and reduction (i.e. both image reconstruction for white beam imaging and more advanced options), as well as implementation of AI/ML tools.

4.3.2 AUGMENTED EXPERIMENT STEERING

The goal is to provide the ILL users with smart tools in order to improve the efficiency of their use of beam time. We have identified two stages in the experiment-to-publication process where numerical tools will contribute significantly: preparing for the experiment and running the experiment.

Experiment preparation will be greatly improved by the use of a "Digital Twin" of the instrument, in which a Monte Carlo neutron simulation is propagated through a 3D model of the instrument, including scattering from the sample and the sample environment. Full ray-tracing models of ThALES, Panther and D11 have recently been developed based on their 3D engineering drawings. The virtual instrument setup is determined using a graphical user interface similar to that available on the real instrument, and sample scattering probabilities are obtained from atomistic simulations. The result is simulated data which can be directly compared to real data, including background effects from sample environment and multiple scattering, allowing such artefacts to be understood and isolated.

Digital Twins can be used not only by users but also by instrument scientists to tackle tasks such as identifying the source of spurious background signals. We plan to incrementally extend the Digital Twin collection to cover many more, and possibly all, instruments at the ILL.

Experiment execution will be optimised by automating the production of meaningful reduced data and then automatically suggesting the next point to measure, based on maximising information, expected sample-dependent physics and accessibility. Two main developments are needed for this:

- *Automatic Reduction* will greatly improve the quality and success rate of experiments by easing the decision-making process on where to measure next, by directly providing the users with meaningful data. The ILL is already working in this direction and has developed a first prototype (consisting of a default reduction workflow with the corresponding infrastructure) to automatically reduce SANS and powder diffraction data. We intend to set up an automated reduction workflow and gradually deploy the existing prototype to all instruments. It will generate FAIR (Findable, Accessible, Interoperable, Reusable) reduced data with metadata integrated automatically in a data catalogue (using SciCat).

- *Autonomous Experiments* combine statistical approaches and reduced data to offer solutions for optimal steering to users in real time. A collaborative project is currently ongoing for implementation of autonomous instrument control on three-axis spectrometers, sampling (Q,E) space and dynamically determining the optimal point for subsequent measurements based on previous data and the shortest time to reach an accessible position. The results of tests run on ThALES were estimated to take less than half the time required for a traditional grid-based method of scanning the same area of reciprocal space. We will provide a tool able to suggest the optimal next point to measure, either from a purely statistical point of view or using known physical information on the system, based on Bayesian statistics and using Physics-Informed Machine Learning (PIML). The ThALES prototype can then be deployed across other instruments.

4.3.3 INTEGRATED PLATFORM FOR ANALYSING DATA

The time and support required for data analysis and fitting often create a bottleneck to the fast and efficient publication of experimental results. Addressing this bottleneck will be a high priority, and we have identified particular needs in the fields of quantum materials and magnetism, life sciences, nuclear and particle physics, as well as for tomography. The Computing for Science (CS) group supports a range of software suitable for the analysis of the neutron data measured at the ILL, including MDanse, SASView, Phonopy, Eurphonics, SpinW and Takin, and the development and support for these codes will continue to be a high priority. Demands in data interpretation extend to simulation using mainstream methods such as Density Functional Theory (DFT) and Molecular Dynamics (MD), which can be used both to prepare for an experiment and to understand the corresponding data. These methods are powerful in well-trained hands and can give outstanding results when used correctly and judiciously.

We propose to consolidate our support for data analysis, interpretation and simulation by creating an Integrated Platform for Analysing Data. The platform will be staffed by scientists with a strong computational and mathematical background to support ILL users, providing software and assisting with data reduction and analysis for rapid publication. The platform will include simulation assistance to support both the general user programme and the Science Hubs. Its members will be encouraged to join the Hubs that correspond to their scientific interest, collaborating to achieve the goals of the Hub. This approach is intended to create close links between computation and experiment, ensuring that the software is compatible with the evolving demands on the instruments and from the user community.

The objective is to provide tools and workflows for data analysis and simulations, hiding the technicalities to improve the users' autonomy with respect to simulations. It will offer Digital Local Contacting services (shared positions between CS and the instrument teams) in order to reduce the load on the Instrument Responsible. We plan to develop simulations for hard condensed matter using either local or cloud-based high-performance computing, employing a workflow prototype using the Hylleraas Software Platform (in collaboration with the University of Oslo). The technical details can be managed via generic user-friendly workflows to facilitate access to computing resources for non-specialists. Simulations for soft matter and biology (such as coarse-grain models and small-angle scattering profiles) can use AI/ML methods to derive information from real data without using analytical models, using an approach known as model-free fitting. This is particularly valuable when classical fitting methods become inefficient as deterministic models reach their limits, e.g. at high poly-dispersity. Such an approach can significantly lower the barrier for non-expert users to extract the desired scientific information from their experiments.

4.3.4 FROM ON-LINE TO REAL-TIME

This is a transverse set of activities that will rely on the development of AI/ML tools to address the most important time-limiting steps in the global data treatment process, deploying these methods to approach real-time data treatment for AI-assisted reconstruction for tomography, Autonomous Experiments and model-free fitting. AI and ML offer powerful and efficient solutions, particularly when handling multi-dimensional data sets, to identify features in data with low contrast and poor signal-to-noise, and to reconstruct images. We will seek to incorporate AI and ML in data reduction processes in collaboration with leading partners in the field. On-site campus collaboration with the ESRF and university digital platforms will be a substantial advantage, as will strong engagement with users who have significant expertise. Collaboration with other major neutron facilities in Europe will help to strengthen the European neutron science ecosystem.

ILL Science Strategy

4.4 COMMUNICATION AND PARTNERSHIPS

- Internal communication within the Science Division will be consolidated with the developments of the Science Hubs and Showcase Experiments.
- The Communication and Public Relations group will publicise the scientific and societal impact of the user programme, Science Hubs and Showcase Experiments to further its programme to promote the public image and societal impact of the ILL.
- The Science Hubs and Flagship Experiments will coordinate and consolidate efforts to attract external funding through grant applications.

The ILL must not only deliver real scientific and societal impact, but must also be seen to do so. Good internal communication will be key to creating and maintaining effective collaborations upon which the success of the Science Strategy will depend. Effective external communication will ensure that the strengths and achievements of the ILL are appreciated by our stakeholders and support political decisions on the future European neutron landscape.

The successful implementation of the new mechanisms in the Science Strategy relies on improvements in internal communication and collaboration. The Science Hubs and Showcase Experiments will serve as forums to foster cross-institute and cross-EPN-campus networks, sharing expertise and knowledge encompassing a broad range of experimental and theoretical methods and applications. Improved internal communication will result in better service to external users, offering closer involvement with local scientists in collaborative efforts and stronger encouragement to take full advantage of the complementarity of neutron techniques.

Effective external communication of the ILL's scientific achievements is needed to strengthen the advocacy of external communities for the ILL value proposition: that our impact on science and society remains both important and strategic and that we are drivers for increasing economic growth. The continuing role of the ILL in the future development of the neutron landscape will depend on the strength of this advocacy.

4.4.1 PUBLIC RELATIONS

The public profile of the ILL is managed by the Communication and Public Relations group. The group has developed and maintains a communication and outreach strategy around the tagline "Neutrons for Society", which is perfectly aligned with the focus of the Science Strategy on areas of societal importance. The group will play a vital role in highlighting the Science Strategy and its progress, and in emphasising the importance of the ILL.

External communication and outreach are currently organised into "experiences", designed to promote the ILL to a broad range of targeted audiences. The experiences are split into three categories:

- Virtual ILL experience – online presence and visibility
- Real-world ILL experience – offline presence and visibility
- Personal ILL experience – direct experience for privileged interactions (VIPs, journalists, industry)

The main actions for each of these categories are identified in the table below.

VIRTUAL ILL EXPERIENCE Enhance the online presence and visibility through a multi-faceted strategy	REAL-WORLD ILL EXPERIENCE Enhance the offline presence and visibility through a coherent set of communication materials and tools	PERSONAL ILL EXPERIENCE Enhance the direct experience for privileged interactions with members of specific audiences
Reorganise and upgrade the public website - Include individual pages for all ILL scientists - Develop a social media editorial strategy and expand to new channels. - Keep a closer and more structured contact with the community - Develop online contents for non-experts - Reinforce appearances in online media	Develop a set of brochures and flyers, including the following: general brochure, neutron technology brochure, areas of impact brochures, industry-related brochure(s) - Improve the setup for ILL visits, both with and without access to the ZAC, including the creation of visuals and outreach tools for wider audiences - Use events as hooks throughout the year, including the participation in outreach events, organisation of on-site events, and road shows.	- Select individuals to act as ambassadors (alumni, ILL staff, users, industry) - Set up tailored visits and events for specific audiences, namely VIPs, industry, journalists, potential ambassadors. Use events as hooks throughout the year. - Support the neutron user community and reach out to potential new communities – push for invited contributions to appropriate conferences, participation in specific events. - Develop the media network and improve media appearances.

The Science Hubs and Showcase Experiments will serve to highlight the ILL's capabilities and to attract external interest and collaborations. They must be widely publicised, with significant coverage and opportunities for external visitors. Further promotion of their goals will be arranged through the organisation of dedicated workshops and meetings. The Communication and Public Relations group will play an essential role in publicising the activities and achievements of the Science Hubs and Showcase Experiments, facilitated by close collaboration with the respective coordinators, who are a natural central contact point. Particular emphasis will be placed on outreach to the media, aiming to ensure that the research performed at the ILL has maximum visibility and public impact.

4.4.2 EXTERNAL FUNDING

A coherent resourcing plan is being developed to support implementation of the Science Strategy. The expansion of the programme for Nuclear Medicine for Cancer Treatment will generate additional income that will support many of the activities of the Science Strategy. Further external funding would expand the reach and impact of the Science Strategy and can be facilitated through the Industrial Liaison Unit and the European Office.

The European Office oversees our participation in EU research and national innovation funding programmes. It acts as a support for the ILL to expand its portfolio of European projects, including both science-based and innovation projects. The activities are currently structured across three key-phases:

• Proposal seeking: identify and create opportunities that align with the ILL's Science Strategy through networking at national and European Commission levels

• Pre-award support: oversee eligibility criteria, budget compliance; coordinate the writing and submission of project proposals

• Post-award support: support and ensure the successful implementation of funded projects, liaise with internal and external stakeholders

The Office has recently been expanded and is expected to be fully self-funded based on the overheads covered by successful grant applications.

The Science Hubs and Showcase Experiments provide ready and coordinated teams of scientists to prepare and manage external funding opportunities. The focus on societal challenges will open new opportunities for applying for funding under Pillar II of the European Commission's Horizon Europe programme. The Hubs will have a strong mandate to actively seek and attract external collaborations, lending themselves naturally to applications for Europe-wide grants for staff and other resources. The European Office will work closely with the Hub coordinators to support the applications for appropriate grants and to assist in their administration.

The award of more prestigious grants, such as those funded by the European Research Council (ERC), will be particularly impactful both in helping to achieve the objectives of the Hubs and Showcase Experiments and in communicating the strengths of the ILL to the scientific and wider communities. Success in applying for ERC grants will depend on effective outreach to collaborators in the user community and high-quality support from the ILL's European Office.

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