Neutron Review 2024
Panel Report

Background

This review was commissioned by STFC in Spring 2024 to assess the impact of the closure of Institut Laue-Langevin (ILL) in 2033 and the opening of the European Spallation Source (ESS) in 2034.

The scope of work for the review was to:

- Review and refresh the science challenges and opportunities requiring sustained access to neutron facilities (as identified in the previous reviews); and identify the unique 'neutron facility' requirements necessary to address the key science challenges.
- Define the available capacity and any loss of unique capability that is likely to occur as a consequence of the changes in the neutron landscape, especially through the closure of ILL.
- Investigate and recommend effective means for meeting the long-term access requirements to neutron facilities for the UK research community.
- As part of the above analysis identify a series of practical actions that the UK community should take to support the provision of the appropriate capacity and capability to the UK community.

The review was sponsored by Dr Alan Partridge, STFC Executive Director, National Laboratories: Large Scale Facilities (at the time of commission). The panel comprised the following members:

- Paul Monks (Chair), Chief Scientific Advisor, DESNEZ
- Jane Nicholson, Executive Director: Research Base, EPSRC
- Jayne Lawrence, Professor and Director of University of Manchester at Harwell
- Paolo Radaelli, Professor of Experimental Philosophy (Physics), University of Oxford
- Pete Dowding, Chief Scientist, Infineum
- Roger Pynn, Professor of Physics, Indiana University Bloomington
- Andrew Barrow, Technical Specialist: Materials, Rolls Royce
- Stephen Hayden, Professor of Physics, University of Bristol

The review panel met in September 2024 and considered a range of evidence including:

1) Status reports from the three in scope facilities and Q&A sessions with each of the three directors.
2) The outcome from a UK Neutron Community Survey performed in June and July 2024.
3) Responses from key stakeholders including the Institute of Physics Neutron Scattering Group, the STFC Physical Sciences and Engineering advisory panel and the STFC Life Science and Soft Matter advisory group.
4) An analysis of the international landscape

1. Introduction

Neutron facilities enable unique experiments to be performed on the structure and dynamics of materials at the atomic scale, thereby providing critical capability for a broad range of scientific disciplines, including physics, chemistry, materials science, biology, pharmaceutical sciences, engineering, and the environmental sciences. Neutron techniques are used to address important societal challenges (in energy, health care, the environment etc.) and provide innovative solutions for industry. The UK neutron user community is one of the largest and most active in Europe, currently supported by access to two world-leading facilities: the ISIS spallation source (the UK's national neutron and muon facility at the Rutherford Appleton Laboratory) and the reactor source at the Institut Laue-Langevin (ILL) at Grenoble.

Over the next 10 years there are numerous significant changes that will impact the European neutron source landscape. The signing of the ILL 6th Protocol by France, Germany and the UK commits to closing the ILL by no later than 2033, and the next generation neutron source, the European Spallation Source (ESS) in Sweden, is currently under construction with full operation of its first phase of 15 instruments expected by 2034. In this changing international landscape, it is important that the UK has a clear strategy regarding continued access and exploitation of appropriate neutron facilities. The intent of this review was not to repeat the comprehensive reviews that were undertaken in 2017 and 2020, but rather to focus on how the UK neutron user community will be impacted, both in terms of capacity and capability, by the ILL closure and wider changes in the neutron landscape. The review focussed on understanding the status and plans of the three neutron sources (ISIS, ILL, and ESS), which are supported by the UK and are extensively used by UK researchers and industry, and considered the implications for the UK community in the context of the wider international landscape.

The committee considered the European landscape and developed several options and key actions for maintaining UK users access to neutron sources through to the 2030s (the transition period) until ESS is reliably running at full capacity and there is more clarity on whether the UK will proceed with construction of a next-generation neutron source. The panel focussed on two key aspects of neutron provision: capacity – the amount of 'beam time' available to undertake neutron-based science, and capability – the range of instrumentation available to undertake neutron-based science.

2. Emerging Scientific Priorities that require Neutron Science

Based on the Neutron Community Survey, the panel found the current provision of neutron sources effectively support both the applied and fundamental science user communities. The neutron source community comprises a very diverse user base, encompassing work across all Technology Readiness Levels (TRLs): from fundamental science to emerging technology, and from applied science to industrial access. A key observation from the review was that neutron techniques are a fundamental scientific tool that underpin research and development across a wide range of subjects and plays a key role in the advance of knowledge and its application. **In light of this importance, the UK must retain and evolve current neutron capacity and capabilities where possible.**

As noted above, neutron science serves a wide variety of disciplines including the physical sciences, engineering, life sciences and the arts and humanities communities. Experiments are becoming more sophisticated, as both the sample and environment become more complex.

Multimodal studies probing the dynamics of a sample have become more prevalent, as reflected by an increase in multi-discipline teams wanting to exploit neutron science at sources such as ISIS.

Across the suite of disciplines supported by neutron techniques there is a growth in demand for *in-situ/operando* studies to probe samples in a functional situation (e.g., a battery discharging). In addition, the user base is expanding beyond those who would consider themselves to be traditional neutron 'experts'. To support these new users, there is a growing need for neutron scattering specialists embedded within facilities who can flexibly partner with researchers, allowing them to integrate neutron science with other techniques to address complex scientific problems. **To support this growing area and maximise exploitation of neutron facilities, it is critical to maintain sufficient staffing and beamtime support as well as state of the art infrastructure.**

Based on data gathered in this review, the neutron capacity needed to support the UK community is forecast to remain comparable with current levels. Advancing neutron capability will be the defining factor in sustaining the community and advancing the applications of neutron-based science. Feedback provided by neutron users in the community survey emphasised the importance of maintaining the provision of current facilities and skilled people capable of adapting existing instrumentation to meet their scientific needs**. As a result, the focus of the next 10 years should be on exploiting current instrumentation, either in commission or in the pipeline, and enhance capability through adaption and evolution, supported by sufficient staffing levels.** Developments in AI and Machine Learning (ML) were repeatedly highlighted as potential 'game changers', capable of revolutionising the exploitation of large datasets generated at neutron sources. Successfully incorporating AI and ML into experimental pipelines also has the potential to increase efficiency of data processing and manipulation, which will be crucial to maximising the effectiveness of the beamtime allocated to the UK neutron community at existing source facilities.

Areas of future growth in neutron techniques

Three key future growth areas of emerging importance for neutron-based techniques were identified by the panel: materials for energy/environment, system level life sciences research and computing and post-conventional electronics.

Materials for Energy and Environment

It is anticipated that neutron use in materials for energy research will continue to grow across a range of different application areas including:

- battery chemistry
- high-density energy storage
- development of novel materials for fission and fusion applications.
- climate change mitigations

Neutron techniques bring particular advantages to evaluating materials for energy through the ability of the probe to "see" light elements such as hydrogen, lithium, carbon, and oxygen – the understanding of which is often critical for optimal performance of energy systems.

Life Sciences

There is immense potential for neutrons to become an important facilitating capability in life sciences research through developments such as:

- faster high-throughput screening techniques for compounds in the biomedical sciences
- enhanced structure and dynamics characterisation capabilities that are needed to clearly understand, and help guide, the development of nanoscale therapeutics

Reactor based neutron sources are also capable of generating medical radioisotopes used to diagnose and treat various forms of cancer. Actinium, thorium and lutetium in particular, can be produced in reactor sources and isotopes of these elements will continue to be in high demand in the future. The next generation of theranostics, used for simultaneous diagnosis and treatment of diseases, will exploit the types of radioactive isotopes produced by neutron sources to advance health outcomes of patients worldwide.

Computing and post-conventional electronics
The neutron's exquisite sensitivity to magnetism positions its scattering and spectroscopy techniques as ideal tools to answer many of the complex questions posed by new classes of technological materials. For example, materials that display properties such as ferro-electric or magneto-resistive behaviour, or harbour exotic magnetic textures such as skyrmions, are currently being used to develop novel memory architectures. Neutron scattering experiments performed on these systems are continuing to provide critical insights into these properties, enhancing our ability to predict, engineer and control emergent phenomena. This new knowledge is helping to drive the much-anticipated 'beyond-silicon' technological revolution, potentially leading to the replacement of conventional semiconductor electronics with faster and more energy-efficient technologies, for example, based on electron spin currents as opposed to conventional electric-charge currents.

Deploying these technologies is also likely to be pivotal for delivering on our global ambitions for quantum computing. One clear goal is to create a new generation of qubits that are protected from decoherence by the intrinsic 'topological' properties of the host material, charting a direct path towards a true general-purpose quantum computer.

Recommendation: Explore ways to integrate transformative developments in AI and Machine Learning, which have the potential to revolutionise the exploitation of data generated at neutron sources, alongside organic development of beamline capabilities.

3. Future Changes in Neutron Capacity

3.1 Baseline Scenario

The panel considered a range of potential options for maintaining neutron provision through the 2030s based on the following baseline scenario by 2035:

- ILL will undergo full closure by 2033.
- ISIS Endeavour will be completed with the new instruments operational by 2033.
- ESS will be working at initial 'full' capacity and capability (15-17 planned instruments) by 2034.

Under this scenario it is anticipated that there will be a ~10% reduction in overall neutron capacity compared to present, based on the number of beam days available to UK users. There is also likely to be a loss of capability associated with the closure of ILL, across a range of techniques and discipline areas including triple axis spectrometry, single crystal diffraction, neutron polarisation, spin echo and imaging. Other areas, such as macro-molecular diffraction, are also likely to be negatively impacted, depending on the length of time between the closure of ILL and effective ESS provision coming online. Further consultation with specific user groups will be required to establish how loss of certain instrumentation at ILL will affect individual disciplines.

Although a ~10% reduction in overall neutron capacity may appear tolerable in the short to medium term, this could translate to a much greater loss of capacity in certain disciplines, or for industry users. Capacity issues may also be further exacerbated by delays in commissioning to the ESS. The panel emphasised that new instrumentation coming online does not necessarily equate to full exploitation, and commented on the rigorous level of optimisation and engagement with facility specialists that is required to enable users to obtain high quality results from neutron facilities.

Recommendation: The UK needs to further investigate the specific capability loss associated with the closure of ILL with regards to scientific disciplines (e.g., triple axis spectrometry, single crystal diffraction, neutron polarisation, spin echo and other specialised imaging techniques), as well as fully understanding the impact on different user groups (e.g., proprietary access for industrial users and policies regarding travel support for top-tier UK experiments).

3.2 Future scenario planning

The panel developed three different scenarios in response to the challenges associated with the loss of capacity and capability identified in the baseline scenario outlined in Section 3.1. All three future scenarios were designed to maintain close to constant capacity through the 2030s, which was recognised as the most challenging period of uncertainty due to transitioning between various neutron sources. Further consideration will be required regarding the longer-term provision for neutron science for the UK community, into the 2040s and beyond.

Scenario 1 – The Three Source Approach: The UK community retains access to short pulse, long pulse and continuous neutron sources via international agreements. In this scenario the UK community would have continued access to ISIS, ESS when it comes online and one or more reactor sources.

- This scenario aims to preserve current levels of neutron capacity and capability available to the UK neutron user community.
- This scenario requires continued access to a continuous reactor-based source.
- A key decision for the UK is whether the UK relies on open international access, as is currently the case for HFIR, NCNR and PSI or whether it seeks to negotiate agreed access with individual facilities (recognising that the UK could also explore mutually beneficial two-way access arrangements).
- This scenario presents the lowest risk to the scientific community due to preserving access to capability at established sources. However, there is a risk that capacity will be further impacted if ESS follows the trajectory of other newly commissioned neutron sources which have required extended commissioning and ramp up time before reaching maximum productivity.

- If this scenario is pursued, there should also be active technology development and work within the community to adapt the scientific applications of pulsed neutron sources to aid an eventual move away from reliance on reactor sources for certain capabilities in the longer term.

Scenario 2 - ESS Enhancement: The UK buys more beamtime at ESS and receives increased access to the facility when it comes online.

- This scenario has the potential to preserve current neutron capacity, however it is likely to result in capability gaps due to the loss of a continuous reactor source and specific associated instrumentation.
- However, this scenario poses a significant risk to the neutron community if ESS does not perform effectively for the first few years of operation due to the complexity of commissioning.
- In addition to the above risk related to delays in ESS reaching full operation, there are additional complication factors within this scenario that need to be considered, such as:
    - The correlation in ultimate investment level and the ability to shape on-going development of ESS science capability to UK needs, when operating in a multilateral management framework.
    - The ability to adapt science capabilities at ESS to those that are needed to match the evolving research interests of the UK neutron-beam using community, particularly where the characteristics of a long-pulse spallation neutron source may be sub-optimal for such needs.
    - The ability to ensure that sufficient levels of proprietary access are available to match the neutron beam requirements of UK industry in terms of timeliness, cost and capability, on top of the demand expected from UK academia.

Scenario 3 - ISIS Endeavour+: The UK increases investment in ISIS to maximise capability and increase capacity for the UK neutron user community.

- This scenario would provide access to short and long pulse neutron sources, keeping investment in ESS at the same rate as currently agreed, but would not provide guaranteed access to a continuous neutron source.
- There is potential that increasing the allocation to UK users could lead to reduced capacity for the international community, based on current operations. However, this could be somewhat mitigated by an increase in the current yearly beam days of ISIS (recognising there are significant limitations on the extent that this could be done; c.10%).
- Increasing beam days at ISIS would require enhanced investment in staffing and operational resource, alongside advancements in computational methodologies to increase efficiency and productivity.
- Further investment in the instrumentation suite of ISIS (in addition to staffing) has the potential to also alleviate capability loss that would occur with the closure of ILL, as well as preserving capacity for the UK neutron user community.

Based on the evidence collected, the panel believed that the <u>neutron user community</u> would favour the 'Three Source Approach' given it presents the highest level of flexibility in terms of neutron source provision and known current capability. The cost of each scenario has the potential to vary significantly when compared to current access agreements; and the panel reflected that this would be a necessary consideration when deciding on scenarios to pursue. In addition to this, the importance of maintaining direct industrial access to undertake proprietary research for UK businesses was highlighted as a key factor in future access strategies. The panel also emphasised that continued investment in ISIS was essential to maintain the UK's national neutron source as a world class facility as part of any future strategy. Also discussed was the need to adapt technologically to have less reliance on a reactor source in the long term.

Whichever scenario is pursued by the UK, there is a risk of losing users within the neutron community during the 'transition phase'. Loss of capacity and access to adequate capability in a timely manner may lead to researchers and industry users utilising alternative techniques to gather data. Of particular concern is the potential loss of new users (e.g., PhD students), who are relied upon to maintain the future pipeline of the neutron community and neutron science in general. **The UK should therefore look to re-iterate its commitment to neutron science as a core strength of its scientific portfolio, ensuring the neutron community is maintained to exploit investment in both current and future facilities.** Potential actions to mitigate this risk include replicating the current model at ILL where travel costs are included in the access arrangement for experiments being conducted at alternative facilities.

Mitigating actions

In order to maintain the neutron community through the transition period and ensure that the UK has the necessary access to the right portfolio of facilities the following actions should be taken:

Timeframe 1: Now-2029

- Actively promote the use of ILL and ensure maximum exploitation for the current level of UK investment.
- Continue to actively support and develop ESS.
- Maintain/increase investment in ISIS.
- Establish the actual capability loss of ILL closure and the anticipated impact that this will have on specific scientific disciplines and within industry.
- Explore funding opportunities to preserve the pipeline of UK expertise in neutron science.

Timeframe 2: 2029-2034

- The UK to establish access arrangements to a continuous source to replace the ILL capacity /capability – this may comprise funded access, open access or bilateral access agreements.
- Invest in technology to replace scientific capability without needing access to a continuous neutron source.
- Commence investment in a next generation neutron source for the UK (in line with the previous two Neutron Reviews that were conducted).
- Continue to support the neutron science community and ensure retention of expertise in neutron science within the UK.

Timeframe 3: 2034+

- Reassess the neutron requirements once ESS is online, and ISIS has been upgraded, noting that technological development may change the provision that is needed.

Recommendation: The UK should implement a "Three Source Approach", to retain access to short-pulse, long-pulse and continuous neutron sources, which should be progressed via the proposed mitigating actions over the next 10 years; recognising that continued investment in the pulsed sources may significantly mitigate the need for access to continuous sources in the long-term.

Recommendation: Funders of neutron science in the UK need to actively maintain and grow the neutron community through the 2030s to avoid erosion during the transition period.

Recommendation: Funders should ensure they have a comprehensive understanding of the requirements of ECRs through the transition period and implement measures to support them where possible.

4. The international landscape

In considering the international landscape the panel advised that it was important to develop an ecosystem approach, without which there is a risk that the European neutron capability could become unbalanced. There has been a marked decline in smaller sources, which can speed up the development of technologies needed to underpin new instrumentation at the larger facilities. The panel noted that new compact neutron sources have the potential to fill that gap and provide a testbed for novel technologies prior to implementation on the larger sources.

The ecosystem approach can only be delivered through developing an effective pan-European strategy. While it was recognised that competition between sources is healthy and can drive innovation, the panel recommended that neutron source providers should be encouraged to take a collaborative approach to delivering European neutron capability. The LENS initiative (the joint initiative of ten European-level neutron facilities) is one mechanism by which this can be achieved; the panel recognised this, advising that the UK should continue to utilise LENS as a conduit by which the European Neutron facilities collaborate informally. However, in some cases there would be value in establishing more formal arrangements (e.g., MoUs or other contractual agreements) between facilities to jointly deliver specific technologies and software based analytical solutions. For example, neutron facilities could choose to formally agree on individual specialisms and appropriate user-access mechanisms to facilitate sufficient capacity in certain techniques for the neutron community – as opposed to duplication of instrumentation and capability in multiple facilities.

The panel identified that there was a need to better recognise the international capital of ISIS and to leverage that capital by seeking to ensure that we are optimising our access arrangements to capability at other international facilities. As part of any new partnering model, it is essential that access for ECRs is fully enabled and remains a priority. In addition, it is also important to ensure that continued industrial access is maintained, and that any revised model does not put in place any additional barriers to UK companies accessing the international facilities.

Recommendation: ISIS, and UKRI, should seek to maximise the benefits to the UK neutron user community by leveraging return on existing international access arrangements and exploring more formal agreements as appropriate. This includes collaborating on both user access and technical development.

5. Closure of ILL

Evidence was provided showing a slight decline in UK users at ILL over the past decade, however there is a clear community desire to extend the lifespan of ILL beyond 2033 if possible and the review panel supported the STFC preference to continue contributing to ILL until 2033 through the extension clause within the 6th protocol.

ILL has recently completed a major upgrade programme (ILL Endurance), delivering thirty new and upgraded instruments and infrastructures. The panel commended ILL's current operations, remarking that the facility is at the highest level of capability and capacity it has ever delivered. This facility needs to be championed in the remainder of its operational lifetime within the neutron user community to ensure maximal return on investment for the ILL and its funders. To maximise the UK's own current investment in ILL and fully exploit the newly upgraded facility, the UK neutron community and its funders should explore increasing PhDs and fellowships that will utilise ILL neutron capability.

In addition to fully utilising ILL whilst it remains operational, the UK should maximise training opportunities at the facility to ensure neutron scattering expertise is passed on to the next generation of instrument scientists. While there is already a large exchange of scientists between ILL/ISIS/ESS, more could be done to ensure the mechanisms in place have the necessary security and flexibility to maximise the benefits for those involved. Concerns were raised about ILL potentially losing key staff as the proposed closure date becomes nearer due to uncertainty over long term career ambitions, and thus impacting the quality of science produced by the facility. The UK representatives for neutron science should work with ILL to scope possible mitigations to avoid this. The panel speculated on whether joint staffing contracts between ILL and other facilities could be introduced to retain key experts within the neutron community in the future, for instance.

Recommendation: The UK should maximise return on current investment in ILL during the remainder of its operational lifetime and accrue expertise within the UK neutron community, via sponsorship of placements at the facility for UK based students and fellows.

6. Summary findings

- There is a long history of neutron scattering in the UK and this continues to be an area of strength in our research and innovation landscape. The review found there to be a continued demand for neutrons by the UK community and a strong drive to further develop capability in neutron science.
- Three scenarios were identified by the panel to mitigate the expected loss of neutron capacity and capability due to ILL closure. These were: maintaining access to three different sources (short pulse, long pulse and continuous reactor), increasing investment in ESS, and increasing investment in the UK's own neutron capability (ISIS).
- Neutron science is evolving quickly, but innovation at the neutron sources in the scope of this review continues to meet the growing needs of the user base.

- ISIS is a truly world class national facility, and it is important to continue to invest and grow ISIS to maintain the UK's national capability in this area. This will provide the UK with a higher level of resilience to fluctuations in international neutron provision.
- The success of neutron science relies upon the effective funding of skilled people to best exploit the instrumentation and resulting data. Maintaining the balance of investment in people, infrastructure and data exploitation will be critically important through the transition period (ILL shutdown and ESS coming online).
- There is a need to maintain a lively engaged science community through the transition period and this will require the balancing of investment between the facilities and the science programmes of the broader neutron-using community.
- There is a substantial opportunity to better exploit data by incorporating AI and Machine Learning techniques into neutron science. This will be crucial to mitigate the increased demand of the neutron user community at every neutron facility.

7. List of Recommendations

Recommendation 1: The UK should implement a "Three Source Approach", to retain access to short-pulse, long-pulse and continuous neutron sources, which should be progressed via the proposed mitigating actions over the next 10 years; recognising that continued investment in the pulsed sources may significantly mitigate the need for access to continuous sources in the long-term.

Recommendation 2: The UK needs to further investigate the specific capability loss associated with the closure of ILL with regards to scientific disciplines (e.g., triple axis spectrometry, single crystal diffraction, neutron polarisation, spin echo and other specialised imaging techniques), as well as fully understanding the impact on different user groups (e.g., proprietary access for industrial users and policies regarding travel support for top-tier UK experiments).

Recommendation 3: Funders of neutron science in the UK need to actively maintain and grow the neutron community through the 2030s to avoid erosion during the transition period.

Recommendation 4: Funders should ensure they have a comprehensive understanding of the requirements of ECRs through the transition period and implement measures to support them where possible.

Recommendation 5: The UK should maximise return on current investment in ILL during the remainder of its operational lifetime and accrue expertise within the UK neutron community, via sponsorship of placements at the facility for UK based students and fellows.

Recommendation 6: ISIS, and the UK, should seek to maximise the benefits to the UK neutron user community by leveraging return on existing international access arrangements and exploring more formal agreements as appropriate. This includes collaborating on both user access and technical development.

Recommendation 7: Explore ways to integrate transformative developments in AI and Machine Learning, which have the potential to revolutionise the exploitation of data generated at neutron sources, alongside organic development of beamline capabilities.