The ISIS Endeavour Programme – Summary of User Community Meetings

July 2021

Contents

Summary

Endeavour is the programme of new instruments and large instrument upgrades that is anticipated at the ISIS Neutron & Muon Source over coming years. The programme consists of around 9 projects which aim to enhance ISIS' capacity and capability to deliver science in three key areas: clean growth; biosciences and health; materials for the future. This report summarises the outcomes of three user community meetings held in July 2021 which focused on the potential of the proposed Endeavour instruments within these three science areas.

The three meetings were held via Zoom, and were attended by a total of 231 unique participants, with 70 attending more than one meeting.

The presentations of the instruments by user community 'champions', together with comments in discussion groups and in the final plenary sessions, showed the strong support of the community for the Endeavour Programme in general and the specific projects relevant to their science. New science areas that the capabilities of the instruments would open up were highlighted for each project, with strong relevance to the three meeting themes and to new communities that would benefit. Uniqueness of the instruments and their capabilities compared with those at other sources were highlighted.

Sample environment provision was a recurring theme, and in particular the need to integrate this within the Endeavour Programme if maximum benefit is to be gained from the new instruments. Creating a specific sub-project within the overall Programme to look at sample environment provision is a suggestion from the meetings.

The importance of high throughput, user-friendly analysis software to make the most of high data rates was a recurring comment, and instrument projects are being asked to highlight their data analysis needs. Increased use of simulation and modelling to enable understanding of more complex systems was also noted.

The provision of appropriate staff support was noted a number of times. As experiments become increasingly complex, additional scientific and technical effort is needed to prepare and run experiments, and analyse (and model) the subsequent data.

Description of the user meetings

The Endeavour Programme has been developed over a number of years, and the projects have been presented to the user community in a variety of ways (for example through the annual UK Neutron & Muon Science and User Meetings, through individual group and technique user meetings, through the ISIS User Committee, through discussions between users and instrument scientists). The Programme has also been discussed at length by the ISIS Science Advisory Committee and the ISIS Facility Board.

A series of user meetings was held in July 2021 (virtually, due to ongoing Covid restrictions). There were several aims of these meetings:

- to update the user community on the Programme
- to continue to explore the scientific possibilities that the proposed instruments would provide
- to receive further community feedback on the projects and their science

- to explore additional aspects (such as sample environment or software) that would be necessary to fully exploit the new instruments.

Clean Growth **Thurs 1 July 2021**	**Biosciences & Health** **Thurs 8 July 2021**	**Materials for the Future** **Thurs 15 July 2021**
HRPD-X Stephen Skinner (Imperial)	*LMX* Peter Moody (Leicester)	*Wish-2* Paolo Radaelli (Oxford)
SuperMuSR Eddie Cussen (Sheffield)	*Sandals-2* Lorna Dougan (Leeds)	*Mushroom* Andrew Goodwin (Oxford)
Tosca+ Paul Collier (Johnson Matthey)	*Osiris+* Maria Paula Marques (Coimbra)	*SuperMuSR* Stephen Blundell (Oxford)
Sandals-2 John Holbrey (Queen's Belfast)	*SANS / reflectometry smaller projects* Sarah Rogers & John Webster (ISIS)	*Tosca+* Sihai Yang (Manchester)
Osiris+ Paul Collier (Johnson Matthey)		*HRPD-X* Emma McCabe (Durham)
e-map Harry Coules (Bristol)		*LMX* Paul Saines (Kent)
Wish-2 Paolo Radaelli (Oxford), Sihai Yang (Manchester)		
107 unique attendees	***80 unique attendees***	***134 unique attendees***

The Endeavour instrument projects presented at the three user meetings, together with their user community 'champion'.

Three meetings were held based around the three science topics of clean growth, biosciences & health, and materials for the future. Each meeting consisted of presentations on relevant Endeavour instrument projects given by user community 'champions', followed by breakout sessions when the instruments and their science could be discussed in more detail. Each meeting then ended with a short report-back from each breakout session, and then general discussion. Talks from the meetings by the user community members are available on the ISIS website, and the main points from the breakout discussions are captured in this report.

General comments from breakout session discussions

Reports from each breakout session are given below. Common themes arose between the sessions, and between the three meetings:

- **Science benefits:** All groups could identify science benefits that the new instruments would generate, both for existing communities using the relevant technique and for new communities that additional capability would attract.
- **Uniqueness and complementarity:** Groups frequently noted where proposed instruments would be complementary to others at ISIS and provide unique capabilities when compared with instruments at other sources.
- **Data rates, beamtime allocation**: Increased data rates provide benefits for more rapid measurement times, as well as enabling smaller samples, more dilute or lower-scattering systems and enhanced parametric studies. More rapid measurement times may benefit

from different ways of allocating beamtime such as shifts, and increased use of Xpress measurements.

- **Sample environment:** A key enabler discussed by many of the groups was the area of sample environment. In particular, the new instrument capabilities would enable greater use of in-situ, in-operando, real-world conditions measurements, more extreme sample environments (pressure, high voltage), combining neutron measurements with other techniques simultaneously, developing gas-loading, new magnets, etc. Groups noted that development of SE equipment would strongly benefit from being included alongside the instrument development so that these capabilities are ready when the new instrument comes online and are available to fully exploit the new instrument abilities. Sample changers will become more important for data rates enabling higher throughput experiments.
- **Software for data analysis:** It was noted that more rapid counting times require greater ability to analyse data during experiments, and that data analysis should enable high throughput and be user-friendly.
- **Modelling and simulation:** Modelling of more complex systems will become more important, and how simulation and modelling capabilities can be enhanced for users was raised.
- **Labs and deuteration:** The importance of ISIS labs for sample preparation and characterisation was noted, including the need for deuterated samples. Links to science capabilities across the RAL campus were noted for some instruments.

The following pages give the more detailed points from each breakout session in each meeting. Breakout sessions were given a suggested structure to aid discussion:

1. Science
Do you consider that the instrument will enable valuable science within the relevant research area? Can you see it meeting your science needs in the future? Are there any science opportunities that we're missing? (Thinking about up to 10 years from now).

2. Enabling areas
Are there additional areas (software; sample environment; support labs; etc) which would need to be developed or made available to ensure maximum science benefit is gained from the proposed instrument?

3. Community
Is there an existing community that will take advantage of the proposed instrument? Will the instrument attract new communities both academic and industrial?

4. Wider fit
How does the proposed instrument fit within the current / future ISIS instrument suite? Does it provide complementary capabilities? Does it enhance the overall ISIS capabilities in appropriate areas? What about world-wide – will the instrument be competitive with those elsewhere?

5. Any other comments
Any other matters related to the instrument that the community would like to comment on.

Breakout Session Summaries

Clean Growth

HRPD-X

Science case

Our champion (Prof Stephen Skinner, Imperial College London) highlighted the key features of the proposed HRPD-X upgrade:

- larger detectors area
- improved capability at longer d-spacings
- increase in detectors coverage (potential increase of 5X in count rate)

The user community will benefit from a revamped instrument which will enable to tackle increasingly complex samples and environments allowing further in situ and operando capabilities (more rapid measurements).

Breakout session

The following points were risen during the discussion:

- Extended detector coverage and higher resolution at lower banks will allow the study of larger unit cell materials.
- The increase in count rate and the introduction of collimation vanes and of a radial collimator will allow “time-resolved” in situ experiments with complex sample environments.
- Some of the users pointed out that the development of different sample environments should go hand in hand with the upgrade (often “retrofitted” sample environments do not lead to successful experiments).
- The HRPD-X lab with allocated sample preparation facilities will facilitate experiments. The dedicated lab is well received by the community.
- The upgrade will change the way we collect data and perform experiments, meaning that more and innovative access routes might be required (ESFR shifts model, allocated time module, etc.).
- HRPD-X will enable new science areas, complementing GEM/Polaris and WISH.

Takeaway

The user community welcome the introduction of features that will enable the study of increasingly complex (and smaller) samples with opportunities to develop new sample environments to probe kinetics, reactions, phase behaviour, etc. of energy-related materials under in operando and real applied conditions.

SuperMuSR

1. Science

The group noted that muon studies of energy materials have moved on from looking at precursor materials to looking at functioning devices. This increases the rate demand because the active volume of the sample is smaller and the measurements can be parametric. Muons are particularly useful for looking at layers within a device so tuning of depth resolution would be particularly valuable, as would the smaller spot size compared to other ISIS instruments - even smaller would be even better. One of the users noted that the extra flux and frequency response from pulse slicing would be particularly useful for light perturbation of photovoltaics and delivering light from the HiFi laser could be useful. The extra frequency response could also be useful for some studies of semiconductors, hydrogen storage materials and green chemistry.

The group broadly agreed that SuperMuSR would meet foreseen science needs in future and suggested that some more control over beam parameters would improve its capability in studying layered devices.

2. Enabling areas

Software: Wimda needs to be sustained going forward, MANTID still needs work. Analysis capability is a possible gap in computing capability. Mac version of MANTID is unstable and clunky

SE: broadly good equipment at ISIS at the moment. Characterisation is excellent in terms of capacity and support.

Computational modelling: Simulations of muon within sample and its effects on the measurement, better coordination of computational support for users, making modelling easier for users to do themselves. These things are already done sometimes but increased use would increase the benefits of the proposed instrument.

3. Community

Battery groups use this technique without being muon experts. Seem as a tried and tested method in battery research. There is a long history of industrial use. As the technique has become more established and widely known the community has grown and seems likely to grow further.

4. Wider fit

Does things we already do but better in this science area. The improvement will exceed an order-of-magnitude in counting rate over both ISIS and all other muon sources. The improvement in frequency response extends capability to areas and communities we don't currently attract. Here the improvement covers a useful level of resolution for this science area with a significantly higher counting rate (~2-5x) than at continuous muon sources that have even higher resolution.

Osiris+

1. Science

The group was convinced that this upgrade will enable new science on Osiris. Through higher flux faster data acquisition is possible, which is an important argument for industrial users. QENS-studies of non-hydrogenous ions in the field of battery materials will benefit particularly and push this field. Diluted systems are becoming more and more important in studies for catalysis applications, where the drive is towards less and less precious materials to be involved.

2. Enabling areas

Instrument upgrades must be accompanied with support from sample environment. More in situ/operando experiments will be expected. Further additional measurement methods like Raman and DSC will need to be integrated more routinely. With the increased flux data analysis must adapt to a higher through-put and in a user-friendly way for the occasional user. The combination of QENS data analysis with MD simulations should be further enabled. The possibility to use AI in data analysis should be explored.

3. Community

Beyond the traditional QENS community users of the low energy spectroscopy community will benefit and be attracted by the increased flux on Osiris. In the field of battery materials users from the Faraday Institution might be encouraged to use QENS as a tool to improve their materials.

4. Wider fit

The primary upgrade for Osiris will deliver new capabilities to the QENS user community and will make Osiris the QENS workhorse at ISIS for the next decades. With this primary upgrade and the concurrent upgrade of the secondary spectrometer Osiris will remain competitive internationally in the foreseeable future.

5. Any other comments

It was stressed that the upgrade project should be seen as an essential upgrade to the ISIS instrumentation to remain competitive in an evolving international neutron scattering landscape.

eMap

1. Science

Higher flux enabling more interesting in situ measurements. Some identified science areas that could benefit from this includes in operando characterisations of the stress distributions and deformation behaviours of new materials for nuclear and offshore wind industry. There was also a great emphasis on additive manufacturing process optimisation using eMAP. For e.g. we could measure in situ the stress in the build during additive manufacturing. In addition, the higher flux may present the flexibility of rapid measurement services for industry at eMAP.

There is a shift in focus of studies in the nuclear field. Within nuclear the focus has shifted from 'life extension of nuclear facilities' to new nuclear capabilities like Gen4 and fusion.

2. Enabling areas

More angular detector coverage. In situ measurements at eMAP will benefit from extra detector coverage to study texture in materials. Nevertheless, the higher angular coverage may limit sample area. Therefore, removable detector banks should be explored.

Extreme sample environments for in situ manufacturing techniques. We should design the instrument to handle extreme environments such as high voltage effects from a welding rig and resistance or how to handle powder materials dispersing from an additive manufacturing rig placed on the sample stage.

Gleeble (an extreme environment thermomechanical rig) would be a brilliant addition to eMAP if we could incorporate it onto the instrument.

Transmission measurement capability at high spatial resolution (for e.g. using the MCP detector currently available at IMAT) will be useful.

SANS capability should be considered for eMAP.

3. Community

The existing engineering community will definitely benefit from the increased flux from eMAP.

The texture mapping capability is particularly interesting for geomaterials. This is particularly interesting in terms of carbon capture technologies.

Increased capacity on strain scanning instruments would enable greater use of Express and Rapid Access proposal access routes. In addition to benefits for the existing user community, this could potentially allow the targeting of application areas such as engineering forensic and failure analysis where the need for faster turnaround times has so far hindered uptake.

4. Wider fit

eMAP is currently not developed to pursue imaging capability. One of the primary requirements is to address the oversubscription for diffraction measurements from industry/academia. Furthermore, eMAP may not be competitive in terms of flux compared to other imaging instruments. However we must explore imaging possibilities on eMAP during the design phase.

Wish-2

1. Science

- WISH is world leading and WISH-II will further enhance ISIS capabilities in the domain of clean growth.
- One of the new key science areas we can expect to be undertaken on WISH-II would be moving to more complex molecules in the guest-host gas loading experiments compared to what is done now. At the moment, only small molecules such as CO2-C3D3 and so on where deuteration is not always possible (this would be enabled with polarisation) is being looked at because of the very limited amount of beamtime on WISH. For example, experiments on biomass systems are currently undertaken at Diamond but they suffer from very small changes in diffraction pattern (just about visible because of the size of the molecule) but this would be much better done with neutrons.
- Gas loading experiment on SX specimen. This is also not done at the moment on WISH due to the lack of beam time availability. Users have to choose the more “simple” and rewarding and higher througput powder experiments but single crystal diffraction would reveal finer details as well as allowing other samples to be studied. The gas-loading experiments on single crystals also have important advantages in terms of equilibration time and data quality and they are likely to be a game changer for the field for some particular experiments.
- A question has been raised on how to balance single crystal experiment and powder experiments.
- Ammonia synthesis with in-situ experiments is also an avenue to explore.
- Another type of experiment that are not taken into account in the science case are electro-catalysis experiment on MOF thin films (usually 1μm thickness, doable on WISH-II).

2. Enabling areas

- Improved sample environments for more efficient gas loading and equilibration. At the moment most of the beam time for gas-loading experiments is “wasted” for thermalization and equilibration.
- High pressure loading is very important in the field, and whilst there has been some prototype experiments, sample environment development is needed. The potential turnkey system iSorb from AntonPaar (used in many labs) would be a most welcome addition to the S.E. suite in that respect.
- A new gas loading system for single crystal experiments (much smaller and needs to rotate).
- Clearly, funding is needed for sample environment developments. Can this be joined with the Endeavour funding bid?

3. Community

- The existing community, which is strong and publishes widely, underlined the need of sample environment developments.
- The community requires more complex experiments involving gas loading on SX, high pressure loading and electro catalysis experiments on thin films. This would likely further increase the community.

4. Wider fit

- There is a question on how to balance the SX and powder experiments between the instruments. When it is not obvious (clearly single crystal or polarisation), proposals to both?
- How does LMX fit into the picture?
- WISH-II was discussed within the context of ESS and SNS and it was shown that due to either the specific characteristics of the pulse, WISH-II will be very competitive with the best planned instruments worldwide.

SANDALS-2

Science:

- Recognition SANDALS is world leading instrument, but count rate not acceptable. Amount of data/samples required for a high impact publication has increased so instrument needs to match that.
- Could allow important fundamental studies of solvents that perhaps require a structural series (e.g. different aromatics) to have importance/impact in the field.
- Allows fundamental studies of deep eutectic solvents and Ionic liquids – key benefit of these systems is properties change with composition, therefore a series of a relatively large number samples is required.
- More structural data on liquids and solutions can help it underpin computational work.
- More possibilities with smaller samples (difficult/expensive to deuterated) or possibilities with containerless techniques to study crystallisation for example
- Higher sensitivity also important for low concentration samples.
- Higher Q resolution important where Bragg scattering is a minority for the sample e.g. telling if a sample has actually melted or crystalline inclusions in glass. Also important for nanoparticles and crystallisation in confinement.

Enabling area:

- D-LAB very important: More samples, but potential to utilise smaller sample sizes
- Sample environment support very important, particularly for *in-situ* and *operando* measurements.
- Increased capacity to analyse more samples required from software too: Dissolve, GudPy projects important.
- Will we need a bigger sample changer? If so do we need to consider this in the design of the vacuum tank?

Community:

- Current demand is to some extent self-regulating – No one wants to do an experiment for more than a week. So it’s expected existing community will use the opportunity to run more samples/state points. NIMROD currently being used for experiments that could be run on SANDALS-II.

- New communities in hydrogenous solids/crystallisation (90 deg bank important here) and time resolved studies for *in situ/operando* experiments.

Wider fit

- Upgrade further differentiates SANDALS and NIMROD: SANDALS has better resolution and decreased inelasticity effects (for near-intermediate order in H containing samples), NIMROD has the ability to look at wide lengthscale range.

Other

- Increased sample throughput would require increased time for users to prepare samples and monitor the data from the ongoing experiment. Therefore larger experimental teams may be required. The increased throughput also brings in the possibility of studying a single system (7 samples for binary system) as a short Xpress/Rapid access (mail-in) experiment, however this would require increased resourcing at ISIS to run effectively.

Biosciences & Health

SANS and Reflectometry smaller projects

The breakout session aimed to answer 4 specific questions. The response from the group are detailed below and considered 4 projects: The SEMSANS-SANS upgrade to Larmor, the focussing SANS upgrade to ZOOM, the development of a USANS instrument for ISIS and the upgrade of CRISP to a reflectometer with lamellar diffraction capability.

1. Science

The SANS projects outlined compliment and extend the existing scientific capabilities of the existing ISIS SANS instrument suite. These instruments already enable a huge breadth of studies to be undertaken which are of both academic and industrial interest and align with the UK governments grand challenges.

The move towards the study of multi-length scale problems will enable the investigation of more industrially relevant and “real-life” systems while maintaining and extending the range of more traditional problems that may be probed.

The upgrade of CRISP to enhance its reflectometry capabilities and to enable lamellar diffraction (LD) from horizontal samples will particularly provide new opportunities for the study of systems relevant to health and ageing. The problems studied with the LD technique typically have a strong link to industrial or clinical questions and there is no reason to believe that this will change significantly over the coming decades. By enhancing the reflectometry capabilities of the instrument and bringing its performance up to modern standards it will also be possible to enable further growth of the reflectometry community which already studies a wide range of science relevant to industry and academia that align with the UK governments grand challenges.

2. Enabling Areas

The provision of deuteration facilities is vital to the success of the soft-matter and bio-science programs at ISIS. Either through the production of materials at the facility itself or through the bulk purchasing of commercial components there is and will remain a need to provide the community with high quality materials that will enable them to perform the best experiments to exploit the unique capabilities of neutron scattering.

The ISIS soft-matter and bioscience community benefit from a wide range of bespoke sample environment equipment managed by a dedicated team of scientists and technicians. The ongoing maintenance and development of such equipment is crucial to the success of experiments. As complexity and new experimental demands increase the importance of a continuing program of development of hardware and software to run the apparatus will grow.

Linked to a sample environment program is the need to develop more sophisticated methods for reproducibly producing and manipulating samples thinner than 1mm for SANS and to better enable cleaning of sample holders. The existing quartz cells work extremely well but are expensive and difficult to clean. Breakages are common and the task of filling and cleaning cells is intensive and time consuming. Flow through methods have been used but significantly increase the required sample volumes which is extremely undesirable when sophisticated deuteration is required. A similar development is required for reflectometry where complex sample preparation can be the limiting step in experiments.

A dedicated preparation area close to the instruments will be required for the ongoing success of the bio-membrane program to be maintained. This will be become more of a problem with the need to manufacture and manipulate samples for lamellar diffraction which will require more time and space due to their complexity and long equilibration times.

Ongoing development of data analysis and reduction software is required to enable the analysis, modelling and interpretation of multi-length scale data. Existing codes require extension to enable simultaneous analysis and to provide additional corrections for effects such as multiple scattering which become stronger with increasing length scales.

A continued detector development program is needed to provide optimised detectors for both lamellar diffraction and SEMSANS-SANS. The existing wavelength shifting fibre technology has the potential to provide suitable pixilation and count rates at a reasonable cost but has the disadvantage of reduced detection efficiency when compared to ^{3}He technologies.

The LD, SEMSANS-SANS, ZOOM Focussing and USANS development programs would all benefit significantly from additional scientific, engineering and technical staff time being made available through additional recruitment in the science and support teams. The demands of the user program and other activities strongly limit the time that can be dedicated to development activities. In addition, the provision of funds to continue development and testing is uncertain making it difficult to plan.

3. Community

Is there an existing community that will take advantage of the proposed instrument? Will the instrument attract new communities both academic and industrial?

There is already a demand from the existing SANS community to probe larger length scales across a broad range of science themes. The bio-science community frequently make use of SANS2D in its 12m configuration which allows it to explore the largest structures. The provision of focussing on ZOOM will enhance this program further broadening industrial and academic interest.

There has been a demand to exploit the SEMSANS-SANS setup developed by R. Pynn et al at Indiana University which has led to the almost annual transportation of the group's equipment to ISIS for a series of experiments. As with the ZOOM focussing the provision of a unique capability enabling the simultaneous exploration of length scales from 2nm-3μm further broaden industrial and academic interest.

The availability of dedicated USANS instrumentation within Europe has decreased with the closure of instruments elsewhere. The demand for USANS can be linked to the increasing SANS community requirement to explore larger and larger length scale from multi-length scale systems across a broad range of science themes. The large, existing SANS community will enable the support of such an instrument.

The Lamellar diffraction community within the UK is relatively small and would require development. In Europe the community has suffered from the recent closure of the V1 instrument in Berlin and this has led to increasing demand for D16 at the ILL. This will provide a latent community to exploit the instrument. A program of development will be required to grow the UK community and to ensure that the existing community become familiar with the exploitation of TOF for the technique.

4. Wider Fit

How does the proposed instrument fit within the current / future ISIS instrument suite? Does it provide complementary capabilities? Does it enhance the overall ISIS capabilities in appropriate areas? What about world-wide – will the instrument be competitive with those elsewhere?

All the proposed projects expand on the capabilities of the existing ISIS instrument suite. The provision of SEMSANS-SANS will be globally unique.

The Lamellar diffraction capabilities of CRISP will complement the existing reflectometry program studying floating membranes and provide unique global capability to study samples using a horizontal sample geometry which will be an advantage for system that undergo transitions into a fluid phase and cannot be studied with a vertical sample. Monte-Carlo simulations and preliminary measurements suggest that the instrument would be competitive with the existing best in class instruments thanks to the exploitation of TOF. The project will enable the initial development of an internationally competitive program prior to a potential further bid to upgrade the front end of the instrument with guides and more open collimation that would further increase the available flux on sample.

The ZOOM focussing program will provide an instrument with unique global capability to explore a simultaneous q range wider than anything available elsewhere. This will require the fast aperture component of the project to be successfully deployed. Without this the competitiveness of the beamline will be reduced for kinetic studies.

It is important that any USANS instrument must be guaranteed to perform extremely competitively with existing instrumentation at ANSTO, NIST and SNS. The flux limited nature of the technique is key to this requirement and long counting times already limit the application of the technique when compared to traditional SANS. Monte-Carlo simulations indicate that an instrument can be constructed that will be competitive with the best in class instruments at ANSTO and NIST but in order to do this a number of compromises have been made in the design when compared to existing instruments. This is why it is key to ensure that simulations of performance are validated prior to developing the case for a new, dedicated instrument. If the simulated flux is reduced by factors of as little as 2-4 the instrument would become non-viable. The project to develop a small scale test setup is crucial to ensuring that simulation matches actual performance and will also serve to highlight any significant problems with the proposed full instrument design.

Osiris+

1. Science

Yes, a highly desirable upgrade for Osiris! The increased flux will enable to run 1) samples in a shorter time and 2) samples of smaller quantity, which might be essential for biological studies. In particular the flux increases will open up studies of more real samples (as opposed to model systems), especially those of medical relevance (eg. Cells, tissues) where sample sizes are much smaller than the traditional QENS sizes. In addition, diluted samples which are often nearer to a practical application, and which typically require post processing analysis such as the subtraction of the solvent signal, will be possible. The application of neutrons in the biosciences exploits the contrast between H and D, and in many cases studies of deuterated samples are hampered by the small amount of available sample material and a decisive increase in flux is crucial.
The availability of higher flux means shorter measurements and thus more parametric studies. This could open more QENS studies in food science in the future, which could have potential industrial impact.

2. Enabling areas

For experiments in the bio area, well maintained and staffed bio and deuteration support labs are essential. In addition, data analysis software should be made more user friendly (for the non-physicist users) and software to integrate molecular dynamics simulations into the data analysis, such as MDanse, should be fully developed. Finally provision of additional experimental probes, like Raman and DSC should be integrated into the QENS experiments.

3. Community

The proposed upgrade will provide gains to the current user community. New avenues for QENS activities for the future identified include the study of air pollution and its effects on cells, food science.

4. Wider fit

Osiris is the QENS workhorse instrument at ISIS. The proposed Endeavour upgrade of the primary spectrometer, in combination with the on-going upgrade of the secondary spectrometer, will keep Osiris competitive amongst all other backscattering spectrometers of its type for the foreseeable future.

Sandals-2

Science

- The upgrades as presented opens up potential for studies on complex multicomponent systems, whereas before the user community may have chosen (or been forced) to pick safer science options (e.g. only considered binary systems, single concentrations etc.)
- Short run times could potentially open up the doors for more fundamental science proposals to come in to the instrument – typically applied science gets the majority share of beamtime, but increases in flux / decreases in counting time could allow shorter, quick-

access experiments that are not challenging the frontiers of science, but provide useful data to the community nonetheless.

- Lowering the counting times required on samples permits better handling of non-stable systems, e.g. systems that are generally not liquid (or try not be liquid) and where even transferring the sample from the lab to the instrument is a challenge against time. Reducing the time spent idle / measuring on the instrument would be beneficial.
- Smaller measurement times also beneficial for measurement at multiple concentrations (throughput) and biological systems that are “time constrained” (efficiency).
- NIMROD programme would also be affected in a positive way, reducing the number of SANDALS-suitable proposals that are moved across because they would simply take too long on the current instrument.
- Increased flux allowing small sample sizes opens the possibility to use samples containing more expensive isotopes, which would otherwise be prohibited by cost.

Sample Environment

- Complementary probes in the instrument to allow characterisation of sample state would be very useful in order to know that samples have (not) reacted, phase separated etc. during their time in the instrument.
- Design of *in situ* probe capability should be kept as flexible as possible to allow the widest variety of samples to be treated.
- Higher flux would open up possibilities for measurements on small samples, especially in the context of levitation experiments. Similarly, high pressure cells with small internal volumes.
- Silica cells to permit optical probes may be the relevant approach here.
- Capture information from *in situ* probes to get data that users “would measure in their own lab”
- Consider neutron camera (following integration of similar system on NIMROD).
- The DANCE concept addresses some of these issues in the form of a completely new instrument, but some ideas from that could be incorporated in a limited scope into our current instrumentation. For SANDALS one key constraint is the sample tank size and access.
- Higher sample throughput could require a larger sample changer, which would require increasing space within SANDALS sample tank – add a “bucket” below and/or above.

Software

- Keeping the relevant software on track (both data analysis and data reduction) is essential.
- Linking Disordered Materials software with data from relevant probes will be a particular challenge, and probably needs to move beyond classical modelling to an extent.

Ancillary Requirements

- Essential to keep ancillary requirements at the same level as the instrument as we move to more complex systems, and consider their development alongside that for the instrumentation.
- Sample environment to handle *in situ* probes etc.
- Moving to smaller samples, more isotopic samples permitted by faster data acquisition times, increasing capacity in the Deuteration Facility is a key requirement.
- Deuteration Facility needs significant investment in order to be able to keep up with the demands and standards that SANDALS-II and other Endeavour projects will have.
- Should the Deuteration Facility be part of the Endeavour programme itself?

Users

- May need larger teams of people to come to experiments to handle the increased sample prep that goes along with a higher throughput instrument.

LMX

1. Science

- Even if LMX is going to be shared with the chemical crystallography community, this instrument is much needed in the structural biology community, especially in view of the over-usage (and about 3x overbooking) of similar existing instruments in Europe, like for example LADI-III@ILL or BIODIFF in Munich.
- The UK structural biology community using neutron diffraction, up to now has been forced to go abroad, for a lack of single crystal neutron instruments that could host their science, and LMX would enable those studies to be done in the UK for the first time ever, both as finite experiments and as preparation for experiments at other facilities worldwide.
- In structural biology, it is of extreme importance to study systems as close to physiological conditions as possible. This cannot be done at synchrotron sources because the energy of the x-ray beam tends to destroy the systems but neutrons, which have a much lower energy impact, can enable studies at RT and/or physiological conditions as well as studies of charged (or redox) systems without perturbing them.

2. Enabling areas

- In designing the LMX instrument, we are already working on a software project to adapt DIALS, the Bragg peak integration software for macromolecular crystallography widely used at DLS, to work with TOF-neutron data. This software will be ready to go even before LMX will be built and will be able to treat SXD data as well.
- A supporting deuteration lab will be needed to prepare the sample for neutron diffraction. Some capacity is already there at ISIS (with the deuteration lab for small molecules) that could be expanded, but the d-Lab@ILL (and in the future possibly ESS) can also help on specific projects and a synergy with the Franklin Institute or the Research Complex (which has already a protein-production facility for the experiments at DLS: https://www.rc-harwell.ac.uk/research-groups/protein-production-uk-ppuk/) should be looked into.

3. Community

- There is already a UK user community of structural biologists using neutrons at other facilities worldwide, that would primarily benefit from a UK-based instrument compatible with their science, but this community could further expand when LMX is up and running, via student involvement and training of new users. Furthermore a quite large structural biology community is regularly using synchrotron (especially DLS) and could be able to use/move to neutrons if a suitable instrument would be available at ISIS, especially if a close synergy would grow amongst the facilities and labs on the RAL site.
- It is somehow surprising to note that there is not enough involvement of the industrial partners that could be future users of the instrument (Wellcome Trust, IBS, Johnson Matthey…). Who is supposed to look into it?

4. Wider fit

- The addition of LMX to the suite of crystallographic instruments at ISIS will greatly expand the single crystal diffraction capabilities, which at the moment consist only of the SXD instrument. LMX will not only offer an additional single crystal instrument but will complement the range of science done on SXD, extending it to larger unit cells and smaller crystals.
- LMX will be ideally situated at RAL, where it could be an important part of a Structural Biology HUB in synergy with the Rosalind Franklin institute, DLS, CLF and the Research Complex.
- LMX will also complement the ILL instruments LADI-III and DALI because it will separate the Bragg peaks in time of flight, rather than using a quasi-Laue beam, consequently allowing the full use of harmonic reflections, which are discarded in the quasi-Laue technique.

5. Any other comments

- LMX will be using cutting-edge detector technology, that has been developed in-house at ISIS and that has been extensively tested on SXD during normal cycle operation in the last two years. The LMX detectors will be at least three times more efficient, with four times smaller pixels than the existing detectors on SXD. This technology will be used to replace all detectors on SXD before the construction of LMX, which will provide further knowledge on the reliability and performance of such detectors.
- It has been recognised that no formal process exist to involve other facilities on campus in any of part of the Endeavour projects and the few collaborative projects, like for example the “DIALS for neutrons” initiative with the CSD, rely on personal contacts and autonomous funding efforts.

Materials for the Future

Wish-2

- **Sample environment**, especially magnets and whether they will be available on WISH-II (they should be able to, since the tank is non-magetic). **New generation of magnets**, relatively compact, possibly vector. High-Tc 3.5 T, quite compact, does not require big cryostats. However, there is no doubt that the WISH-I geometry is ideal for magnets (and with was designed with magnets of that generation in mind), and there is not much to gain for the additional OOP coverage.
- **Detector technology and associated collimation/SE**, and ‘ideal’ pixel size, keeping in mind that small pixels with a close-in detector will have an impact on resolution for the larger samples and also sample environment/collimator. Also note that it is not very useful to transport neutrons that you don’t use, so the guide should be tailored to the largest sample size.
- **Balance of programmes** on WISH-I, WISH-II and LMX, keeping in mind that LMX and WISH-II will have a lot of similarity. Polarisation analysis quite unique and will add a lot to the science suite.

- **Moderator improvements**, tails, change of charge, temperature. Immediate benefits for users and also long term.

Tosca+

Main topics of discussion:

- Sample environment and support labs,
- Data analysis and computational support,
- New science areas

The increased sensitivity from the proposed upgrade of TOSCA secondary spectrometer will be beneficial across all research areas as it effectively leads to either (or a combination of) faster measurements, smaller samples, or higher statistics. In terms of new science area, the upgrade may allow the study of molecular vibrations in thin films, for instance of semi-conductors, proton conductors or electrodes for catalysis.

A strong emphasis was made on sample environments. Because of the significantly increased flux, the measurement time becomes comparable or shorter than the overhead, which is essentially the time required to cool the sample from room temperature to 20 K. For standard measurements, the obvious solution is the use of a sample changer. For studies that require more complex sample environments, such as gas handling experiments, the situation is more complex. Several solutions were discussed: (1) using a different type of cooling system, or more efficient compressors, (2) using smaller cells that should cool down faster, (3) designing a new cryostat, for instance a two-stick cryostat, or (4) more systematically pre-cool the sample in liquid nitrogen. Clearly this is a concern, and this issue must be addressed in the design phase to ensure that there is minimal waste of measurement time due to overhead.

Another source of overhead is, for catalysis, the reaction time itself. This overhead could be cut down by running multiple reactions in parallel in a dedicated support lab, and then measuring on TOSCA when ready. This would require additional support and the acquisition of additional gas panels, i.e. the expansion of the catalysis lab. More generally, additional support will be required for TOSCA as the experiments become more demanding in terms of sample environments and support labs. Similarly, more staff will be required to cope with the increased output of the instrument.

Finally, data analysis and computing support was shortly discussed. The “endgame” would be to be able to perform the full analysis of the data on site, including simulations. Practically this is not possible as it would require a colossal amount of computing resources. Another point was the use of AI/machine learning to perform an “on the fly” peak assignment analysis based on libraries. This might be beneficial for in situ experiments were decisions have to be made as the first data are measured.

Mushroom

Executive summary:

1) The transformative capabilities of Mushroom were complimented by the user community: “Mushroom will do for inelastic neutron scattering what WISH has done for neutron diffraction.” It will enable experiments in new areas which were not thought to be possible before and it will provide ISIS with a new type of spectrometer which does not exist anywhere else.

2) The excitations group has traditionally many expert users and hence the community is very interested in the technical details of Mushroom (see below).
3) Support capabilities will be important for Mushroom to be successful. This includes new sample environment as for example high-field magnets as well as sample deuteration capabilities.

Comments from users:

"Mushroom provides ISIS with a new type of instrument which currently does not exist neither at ISIS nor at any other neutron scattering facility worldwide. There are very few instruments available which can measure inelastic neutron scattering under pressure or small samples."

"Mushroom will do for inelastic neutron scattering what WISH has done for neutron diffraction." Meaning to enable the study of new areas which were not thought to be possible before. It provides ISIS with a new type of spectrometer which does not exist anywhere in the word.

"Moving from a 1 g sample to something 50 times smaller than that is really transformative for people working in the field of metal-organic frameworks since very often samples can be prepared in very small quantities only."

"Allowing smaller samples to be studied will make Mushroom outperform other neutron spectroscopy instruments."

"The low energy spectrometers at the ILL are the most oversubscribed instruments every year for the last 10 years. Since the research on for example frustrated magnetism which relies on these type of spectrometers will continue for many more years building Mushroom rather sooner than later is of utmost importance."

LMX

1. Science

- The main driver for LMX in the context of small molecule crystallography is access to smaller samples and larger unit cells than currently possible. In the international context this would make LMX a unique instrument in Europe with comparable capabilities in the US at SNS and Japan at J-PARC. The envisaged sample volume would be less than 1mm^3.

- Of particular interest to chemists is the characterisation of interactions involving metal-hydrogen bonds and hydrogen bonding (particularly those involving unconventional types or proton migration) for which the precise geometry can only be obtained using neutron diffraction.

- In addition the ability to obtain crystal structures of hydrogeneous samples without the need to deuterate is a key advantage. Deuteration can at times alter the physical properties of a material due to the isotope effect and is often not possible for systems of interest to the chemical crystallographic community e.g. studies of systems with new organic components.

- Distinguishing neighbouring elements in framework materials such as zeolites.

- Enabling magnetism studies of systems with more complex crystal structures where both need to be able to be refined accurately to address the science problems e.g. molecular magnetism.

- Working with smaller samples would enable achieving higher pressures using a more compact diamond anvil cell for geological samples. For organic molecules, a gas pressure cell would remain adequate for the pressures needed.

- Measuring diffuse scattering in smaller crystals and closer to Bragg peaks will be possible.

2. Enabling areas

- LMX will be a unique instrument for small molecule crystallography in Europe with respect to overcoming limitations in crystal size and unit cell volume.

- This is supported by adapting the DIALS software widely used at DIAMOND to process data from both SXD and LMX. Some degree of automation is desirable, particularly to enable informed decision-making in the early stages of an experiment to assess crystal quality.

- The developments in detector technology based on wavelength shifting fibres will greatly benefit both LMX and SXD pushing the detection efficiency on a similar level as the much more expensive ^{3}He technology.

- It will be important for the instrument to have capabilities for handling at least somewhat air, vacuum and moisture sensitive samples to service the needs of the chemical crystallographic community.

3. Community

- The instrument will be shared with the structural biology community.

- This instrument will also offer the opportunity to engage a much broader range of chemists interested in the structures of molecular and framework materials than currently use ISIS, bringing a new community of users attracted by the ability to tackle more complex structures than are possible using SXD or neutron powder diffraction. This includes researchers, for example, who identify with the chemical crystallography community and more synthetically oriented chemists who use the National Crystallographic Service. Some work may be necessary to grow the small molecule community. It is anticipated that existing users will immediately reap the benefits of LMX in addition to SXD, including materials chemists and condensed matter physics communities. Some users who currently use facilities outside Europe to measure small crystals can do their experiments at ISIS in the future. SXD is undergoing an upgrade with respect to detectors and possibly beam transport optics.

4. Wider fit

- LMX will not only attract new users from the structural biology community but also enable UK users who currently perform their experiments abroad, e.g. at TOPAZ (SNS, US) or KOALA (ANSTO, Australia) to perform these experiments at ISIS.

- The sharing of a neutron single crystal diffractometer between to very distinct communities is rather unique. This enables on the one hand to grow an existing community and on the other hand to attract two new communities of structural biologists and chemical crystallographers, for which there has been nothing on offer at ISIS so far because the systems they are interested in are too complex for powder diffraction and cannot yield crystals suitable for SXD.

- LMX will be a unique instrument providing large scale reciprocal space sampling for samples less than 1mm^3 in Europe for small molecule samples. Similar capabilities exist in the US (SNS), J-PARC (Japan) and ANSTO (Australia).

5. Any other comments

- One of the key developments is software development. This is addressed by adapting DIALS which is widely used at DIAMOND to process data from the macromolecular beamlines as well as the small molecule beamline I19. Some degree of automation is desirable and will be pursued.

- The recent developments in wavelength shifting fibre technology for detectors is overcoming the limitations in previous iterations of LMX. These detectors enable superior spatial resolution of less than 1mm compared to the 3mm currently available on SXD coupled with a detection efficiency close or even surpassing ^{3}He technology at the fraction of the cost.

SuperMuSR

Science

The users were confident that SuperMuSR enables valuable science within this research area and meet their needs in the foreseeable future, by maximising the benefits of a pulsed source while migrating the disadvantages. SuperMuSR will be the next generation of muon instruments at a pulsed source and is likely to be ‘rolled out’ across other pulsed facilities.

It was noted that in this science area the users’ requirements could be summarised as higher statistics, lower temperature, higher magnetic field, smaller samples, and higher pressure. SuperMuSR addresses the first four of these and the resulting technical developments can be transferred to future upgrades of the RIKEN instruments that are better suited to pressure studies. Users asked about measuring small samples, which will be possible with the flypast technique used on other ISIS instruments, and pulsed techniques, which will continue to be available and will benefit significantly from the improved instrument.

Enabling areas

With the much faster counting rates, the users may require faster sample environment such as cryostats that can cool or warm quickly. However, it was noted that μSR is currently statistics-limited so the increased count rate is likely to result in more detailed experiments that take higher quality data that can constrain models that are more advanced. SuperMuSR will use event mode and this could slice up a continuous temperature scan after the experiment. A sample changer may become useful, which would need to work at cryogenic temperatures.

Improved data analysis software may need to combine high frequency data with high rate, long time data, handle large numbers of detectors conveniently, and utilise the event mode data effectively.

Community

The existing community will take advantage of SuperMuSR to give a higher throughput and higher quality data. Users currently needing a continuous source will be able to use it: the combination of good frequency resolution and sub-1K temperatures is currently under-resourced since the closure of LTF at PSI. This will also mean some experiments now done in two parts at ISIS and PSI can be done in one experiment, increasing overall capacity.

Many experiments that are rate-limited and therefore not carried out will now become practical, with shorter counting times. This is particularly important for experiments using pulsed techniques, with the potential to attract new user communities as more complex experiments become feasible.

Wider fit

The instrument is complementary with existing pulsed and continuous instruments, providing a unique combination of frequency response and counting rate. It also increases the range of complementary studies users perform in conjunction with neutron scattering experiments. It was noted that no current instrument elsewhere would provide the counting rates that SuperMuSR provides over its frequency response. ESS has no muons so it is important for ISIS to keep developing muon instrumentation in the European and World context.

Any other comments

No further comments were made by the users present in the discussion session. One user sent the following message afterwards:

“SuperMuSR looks great, I just thought I would email you to say that it is possibly the instrument of most interest to me in Endeavour.

Having been part of the CAMEA/Bifrost proposers for the ESS, and a neutron scatterer, I decided to attend the Mushroom break out session.”

HRPD-X

Science case

Our champion (Prof Emma McCabe, Durham University) highlighted the key features of the proposed HRPD-X upgrade:

- Improved capability (count rate and resolution) at longer d-spacings
- Increase in detector coverage overall (potential increase of 5X in count rate in backscattering)
- Non-magnetic sample tank to allow measurements in applied fields.

The user community will benefit from a revamped instrument which will allow measurements of smaller samples and materials with larger unit cells (complex structures, frameworks, etc.). The increase in count rate, together with the introduction of radial collimator vanes and of a non-magnetic sample tank will allow more complex in situ experiments (kinetics, applied fields, etc.).

Breakout session

- The user community strongly-supported the proposed HRPD-X upgrade.
- High resolution powder diffraction is an extremely important part of the suite of capabilities/instruments available at ISIS.
- The high resolution of the backscattering bank is the flagship characteristic of HRPD (and HRPD-X), and it is fundamental for understanding subtle and important structural features at short d-spacings. However, the user community also require access to the structural information stored at low angle (larger d-spacings) for the study of samples with larger unit cells and complex structures and of magnetic and electronic effects.
- With its expanded and renewed array of detectors, HRPD-X will grant simultaneous access to high resolution diffraction at small d-spacing and high-to-medium resolution diffraction at larger d-spacings, allowing the study of systems which are currently inaccessible on HRPD and/or require complementary experiments on other instruments.
- The introduction of a non-magnetic sample tank will enable important studies under applied magnetic fields.

- The increase in count rate and the introduction of collimation vanes and of a radial collimator will allow "time-resolved" in situ experiments with complex sample environments (applied fields, single crystal, pressure, etc.).
- HRPD-X will provide a more efficient way of investigating materials and will importantly complement the capabilities currently offered by other instruments such as GEM, Polaris and WISH. The community stressed the ongoing need for diverse ecosystem of diffraction instruments at ISIS and ISIS-II in order to address the global challenges being addressed by materials science.
- Members of the user community highlighted the continuing requirement of software development for flexible data acquisition, particular of pixelated datasets (with concomitant large file sizes) for dealing with single crystals, study of anisotropy and texture in powders.
- The value of engaging with industry, particularly as a means of funding specialised items of sample-environment equipment was raised.

Takeaway

HRPD-X will maintain its role as one of the highest-resolution neutron powder diffractometers in the world, while also benefitting of expanded detector capabilities at lower angles and improved beam collimation. HRPD-X will expand on the science opportunities offered by ISIS by complementing the current suite of instruments.