International Review of the IRIS and OSIRIS Instruments at ISIS

Executive Summary

IRIS and OSIRIS support a broad range of internationally renowned pure and applied condensed matter science, covering topics in physics, chemistry, materials and biology. This research exploits the instruments’ capability to probe low energy relaxations with high spectral resolution, and covering a wide range of energy transfers with simultaneous diffraction. Fundamental phenomena include molecular rotations and diffusion, with applications ranging from drug delivery, to energy and functional materials. In many cases data from IRIS and OSIRIS are complemented by those from other instruments, notably TOSCA, and are supported by classical and/or quantum molecular modelling. The user community of IRIS and OSIRIS is strong, with approximately 120 PIs, of whom around 80 are based in the UK. Over the period 2008-2013 IRIS and OSIRIS experiments have led to approximately 130 peer reviewed publications, with an overall ratio of refereed publications to accepted proposals of 0.64. In terms of sponsorship, approximately 40% of all proposals submitted by UK-based PIs are supported by EPSRC grants, and around 5% are involved in programme access. A number of PIs have direct links or sponsorship from industry.

- The panel concludes that there is a very strong business case for QENS capability at ISIS.

In terms of their technical capabilities, there is strong overlap between the two instruments, but OSIRIS currently shows flux gains over IRIS of approximately 3 and 9 times for the PG(002) and PG(004) analyser options respectively. For this reason OSIRIS is identified as the priority for technical developments. In the context of the ISIS TS1 upgrade project, the instrument team have proposed a Phase-1 development of the secondary spectrometer by addition of a Si(111) analyser (£0.6M), to be followed by Phase-2 optimization of the primary spectrometer (£3M). Together these would provide ISIS with a unique cold-neutron spectrometer, distinct from LET for example, at excellent value for money.

- The panel strongly endorse Phase-1 and Phase-2 of the OSIRIS development plan.

Securing the future and sustainability of IRIS, on the other hand, calls for a different approach. We note that since 2010 both instruments have been running at approximately ¾ capacity, due to staffing issues, while ISIS itself has recently been operating reduced cycles for financial reasons. Both issues are likely to be resolved or mitigated in the short- to medium-term, leading to a reduction in the instruments’ oversubscription rates. These currently stand at IRIS 1.52 (2009-13) and OSIRIS 1.39 (2008-2013). For IRIS to be viable, it is therefore essential to increase the user-base. Building on the success of the Xpress access route, the instrument team have proposed a Phase-1 development pathway to increase demand for the instrument by offering high-throughput QENS, with the aim of increasing the rate at which systems can be studied by a factor of ten. This initiative might also serve to increase use in areas such as polymers and biomaterials, though in the longer term a stronger research community in these areas could be further developed through the design and implementation of a FIRES type instrument. Strategies for Phase-1 include the automation and standardisation of sample, experimental and data analysis protocols. This process has the panel’s support, since it is low cost and is transferable across ISIS. When Phase-1 has had time to bed-in, Phase-2 options include upgrade of the existing instrument, or a new build on the beam-line (for example based on the FIRES or ELF proposals). We note that planning for either option would place significant demands on the beam-line staff.
• The panel supports Phase-1 of the IRIS development plan, and suggests ongoing review of Phase-2 options for this beam-line.

Notwithstanding the excellent proposal-to-publication rate for these instruments, data analysis and modelling remain significant issues, and ones that are highlighted in user questionnaires. The introduction of MANTID has the potential to greatly improve accessibility, and integration of the QENS tool-kit within this open-source software is a clear priority. The need for detailed modelling of QENS spectra is also unquestionable, to allow calculation of the neutron observables from time-dependent computer simulations. With this in mind, an ambitious work plan of first-principles and force-field based calculations is proposed as a high priority. Phase-1 requires recruitment of a full-time scientist to be embedded within the IRIS/OSIRIS team, upgrade of the infrastructure, and software development. The aim is to enable modelling studies of up to ten new systems per year. This phase has the panel’s support, though we recommend that the mechanisms for choosing systems and identifying collaborators should be discussed in detail with the ISIS management and stakeholders. In addition, we feel that this Phase should be integrated closely with other analysis/modelling initiatives at ISIS and elsewhere. Phase-2 extends to other HPC initiatives, and we suggest that this should be kept under review during Phase-1.

• The panel strongly supports the integration of the QENS analysis toolkit within MANTID. The panel supports Phase-1 of the proposed development for data modelling, and recommends ongoing review of Phase-2.

Among the other factors that have contributed to the strong scientific performance of both IRIS and OSIRIS, the panel would like to highlight the enthusiastic and knowledgeable beam-line staff, particularly bearing in mind that the QENS team of the ISIS Molecular Spectroscopy Group has recently been down to 3 experimental members of staff. In addition, it is worth noting the excellence of the sample environment support at ISIS, which enables technically challenging experiments to be conducted routinely.
1. Background and Remit

ISIS intends to review each of its instruments after 10 years of operations using an external panel of experts, with a shorter ‘light touch’ review every five years. This review process has started relatively recently, with the first instruments to have an External Review being MAPS, MARI and TOSCA. This current review will focus on the backscattering instruments IRIS and OSIRIS, with a particular focus on QENS at ISIS.

The members of the review panel were: Neal Skipper (Chair, UCL), Bernhard Frick (ILL), Heloisa Bordallo (University of Copenhagen) and Craig Brown (NIST). The review meetings took place from 4th – 5th November 2014, and the panel would like to thank the ISIS management and all the staff involved for their cooperation, clarity of presentations, and timely responses to requests for further information.

The written documentation provided to the panel was very clear and well-structured (exemplary in fact), and contained sufficient detail for us to understand the current instrumentation and its context, the scientific outputs, and the proposed routes for technical developments and their underlying rationale. The oral presentations and Q&A sessions were extremely valuable, since they allowed us to enter into in-depth discussions with the scientific team. We were very impressed by their enthusiasm, and depth of understanding of the technical contexts of their instruments and the scientific drivers. The presentations were: “IRIS: Past, Present and Future”, by Dr Victoria Garcia Sakai; “The ToF-Backscattering spectrometer OSIRIS”, by Dr Franz Demmel, and; “Computer Simulations and IRIS & OSIRIS”, by Dr Sanghamitra Mukhopadhyay.

Our review is structured to address the Terms of Reference provided by the ISIS Management, as listed below, and should be read in conjunction with the briefing paper “IRIS and OSIRIS International Beamline Review” supplied to the panel by the science team.

Terms of Reference of the Review Panel:

To provide the Director of ISIS with a review of the IRIS and OSIRIS instruments, particularly considering the role of QENS at ISIS.

The review should consider:

- The current status of IRIS and OSIRIS in terms of instrument technical capabilities, considering the wider ISIS instrument suite (especially overlaps with LET) and similar instruments elsewhere (including potential QENS instruments at ESS and BASIS at SNS).
- The recent science results from IRIS and OSIRIS.
- The current business case for a QENS activity (e.g. demand; sponsorship of use by UK research councils, overseas partners or industry; breadth of scientific use; overall impact).
- The future of the IRIS and OSIRIS instruments, and the QENS area at ISIS. This may include, but is not limited to:
  - The future science needs for the instruments and for QENS, and the business case for these.
  - Suggestions for technical developments, or new instrument capabilities (including modifications to existing instruments or new instruments), in this area.
- Future needs for data analysis or modelling.
- Other developments or provision which will develop the capacity or effectiveness of IRIS/OSIRIS/QENS studies at ISIS.

- Any other comments the panel wish to make to the ISIS Director.

2. Current Status of the Instruments

IRIS and OSIRIS are high-resolution indirect geometry quasi-elastic (QENS) and inelastic (INS) neutron spectrometers, with long-wavelength back-scattering diffraction capability. They both view the 25 K liquid H\textsubscript{2} moderator on the ISIS Target Station 1 (TS1), and they share the N6 beamline. There is strong overlap between the two instruments, but OSIRIS currently shows flux gains over IRIS of approximately 3 and 9 times for the PG(002) and PG(004) analyser options respectively.

At this point we note that since 2010 the instruments have been running at approximately ¾ of their capacity, due to low staffing levels. This issue is being addressed via recruitment of a 4\textsuperscript{th} member of the team.

**IRIS:**

The indirect geometry time-of-flight spectrometer IRIS has been a fixture at ISIS since it’s commissioning in 1986. With several modifications through the course of its history it is has proven to be a pioneering spallation source instrument for quasielastic (QENS), inelastic (INS) and more recently diffraction studies. The beam is delivered from the decoupled H\textsubscript{2} moderator through a bent natural Ni guide, with a final m = 2 converging guide to the sample position. The workhorse analysers are cooled graphite leading to an energy resolution, dynamic window, minimum and maximum Q of 17.5 \(\mu\text{eV}\), -400 to 400 \(\mu\text{eV}\), 0.42 Å\(^{-1}\), 1.85 Å\(^{-1}\), and 54.5 \(\mu\text{eV}\), -3.5 to 4 meV, 0.84 Å\(^{-1}\), 3.7 Å\(^{-1}\), for PG(002) and PG(004) reflections respectively. An option to run the choppers slower than the source, resulting in reduced flux, can extend the dynamic range. The spectrometer can, in principle, be augmented with a high energy resolution option obtainable using mica analysers, though in practice this option is seldom used due to factors such as low flux and increased background in the hydrogenated mica. The PG capabilities are mirrored on OSIRIS, but OSIRIS gains approximately 3 and 9 times the flux on the PG(002) and PG(004) options, respectively. A set of diffraction detectors set out of backscattering give an added capability of simultaneously measuring diffraction. The versatile nature of the sample environment space on IRIS means that most of the ISIS tailored cryostats and ancillary equipment is suitable for use, excluding magnets due to the proximity of the scintillation detectors.

**OSIRIS:**

The OSIRIS instrument was commissioned between 1996 and 1997, and underwent two major upgrades, in 2002/2003 and 2013. The beam is delivered from the decoupled H\textsubscript{2} moderator through a curved m = 2 super-mirror guide, with a final m = 3.6 converging guide to the sample position. Crystal analysers are cooled graphite leading to an energy resolution, dynamic window, minimum and maximum Q of 25.4 \(\mu\text{eV}\), -400 to 400 \(\mu\text{eV}\), 0.18 Å\(^{-1}\), 1.8 Å\(^{-1}\), and 99 \(\mu\text{eV}\), -3 to 4 meV, 0.37 Å\(^{-1}\), 3.6 Å\(^{-1}\), for PG(002) and PG(004) reflections respectively. By providing for medium resolution for QENS and high-resolution for low excitation inelastic scattering, OSIRIS, allows for a large variety of scientific output ranging from quantum magnetism to dynamics of glass formers and novel battery
materials. Its particular strengths are its fine inelastic resolution 0.032 meV at 3 meV energy transfer and its ability to provide for variable elastic resolution and large Q-range coverage. Moreover, OSIRIS was the diffractometer of choice for solving magnetic structures due to its capability of covering a large d-spacing range, between 0.8 Å and 20 Å.

**Instrument Context:**

These instruments should be viewed from the context of the current ISIS instrument suite and also internationally. Clearly OSIRIS has superseded IRIS in capabilities. Moreover, development of a powerful diffractometer, **WISH**, has made purely magnetic structural studies on OSIRIS redundant. OSIRIS is also facing increasing competition from **LET**, which can outperform OSIRIS in the low energy low Q-range, however this is at the expense of dynamic range and inelastic resolution. Consequently, even though LET has a higher count rate, OSIRIS remains a very strong and highly competitive instrument for the study of low lying magnetic excitations and for the study of hierarchical systems exhibiting a distribution of relaxation processes across time and space.

Internationally, these instruments compete with spallation source based instruments DNA and BASIS that can achieve close to 2 µev and 3.5 µev elastic resolution, respectively, with wide dynamic range. A similar instrument concept to DNA has been developed for ISIS, called **FIRES**. The initial concept was a prohibitively costly long instrument, but with fast choppers this concept could be built in well under 50 m, not much longer than the current IRIS/OSIRIS instruments. Sub-µeV energy resolution is achieved at reactor-based backscattering spectrometers, such as **IN16(B)** at the ILL, **HFBS** at the NCNR, and **SPHERES** at the FRM-II. At the same time, these backscattering spectrometers suffer from the somewhat limited dynamic range achievable with Doppler-driven monochromators in the range ±30–35 µeV. The BATS option on IN16(B) at the ILL will alleviate these problems with an energy transfer range of ±250 µeV that can be tuned asymmetrically.

Designs are under development for low energy time-of-flight spectrometers at the ESS, which could be available for users from the mid-2020’s and beyond. The predicted flux increase on MIRACLES at comparable resolution to the current OSIRIS would be a factor of 200. This factor would be reduced with OSIRIS upgrades as discussed later.

3. **Recent Science Results**

The programme of research conducted on IRIS and OSIRIS is internationally renowned. It covers a broad range of pure and applied condensed matter science, with topics in physics, chemistry, materials and biology.

Recent science on IRIS and OSIRIS exploits the instruments’ capability to probe low energy relaxations with high spectral resolution, and covering a wide range of energy transfers with simultaneous diffraction. Fundamental phenomena include molecular rotations and diffusion, with applications ranging from drug delivery, to energy and functional materials. In many cases data from IRIS/OSIRIS are complemented by those from other instruments, notably TOSCA, and are supported by classical and/or quantum molecular modelling.

**IRIS:**

Studies of nanoporous materials on IRIS have elucidated molecular binding, diffusion and transport in a range of topical substrates including metal organic frameworks (MOFs), zeolites, graphite...
intercalates, and clays [Yang et al Nat Chem 2014; Huang et al PCCP 2009; Lovell et al PRL 2008]. Excellent gas handling facilities have enabled experiments on a wide range of adsorbates, from molecular hydrogen to hydrocarbons. Studies of energy materials include proton conductors and battery electrodes [Miyatsu et al PCCP 2014]. In soft condensed matter and biological systems, water dynamics remain a central theme, with systems ranging from models such as lysozyme to in vivo studies on cells [Gerelli et al Soft Matter 2011; Stadler et al JRS Interface 2011]. Users of the instrument have also successfully investigated relaxations in amorphous polymers, foodstuffs, cements, surfactants, and lipids/membranes, all of which fall within the timescales of the instrument. Overall, approximately two thirds of the IRIS user programme is in chemistry and materials science, followed by physics and soft/biological matter. Over the period 2008-2013 IRIS experiments led to 72 peer reviewed publications, and the ratio of refereed publications to accepted proposals is an impressive 0.72.

**OSIRIS:**

The recent science results obtained from experiments at OSIRIS are striking and cover several research areas as some highlighted experiments show. Particularly unique results were obtained for strongly correlated electron systems [Coldea et al., Science 2010; Stock et al. PRL 2012; Tennant et al. PRL 2012] for which the high energy resolution at relatively large energy transfer of OSIRIS was essential (and with further improvement expected with Si analysers) to measure the position and width of low energy excitations. The diffraction possibility on OSIRIS also led to interesting publications in magnetism and superconductivity [Cortes-Gil et al., Chem. Materials 2011], though the purely diffraction activity has decreased recently due to the operation of WISH. Other examples for important ongoing studies concern the fields of catalysis, battery research and phase change materials, where OSIRIS profits from a relatively high energy resolution, though some of these examples experience the limitations of the present OSIRIS. Improving the energy resolution further and increasing the flux would help to acquire better quality data. After the installation of the beryllium filter, the OSIRIS team has now found a new niche of research that is concentrated in the study of functional materials. Overall, approximately half of the OSIRIS user programme is in physics, a third in chemistry and the remainder in materials and biology/soft matter. Over the period 2009-2013 OSIRIS experiments led to 59 peer reviewed publications, and the ratio of refereed publications to accepted proposals is 0.59.

**Scientific Context and Opportunities:**

The suite of scientific studies conducted on IRIS/OSIRIS should be compared and contrasted with those performed on other instruments world-wide. The US has a wide cross-section of science performed on both HFBS and BASIS, with several papers being produced through the natural complementarity of HFBS having the higher resolution. The latter studies concern water, biomolecules and polymers, where pushing towards the slowest relaxation times is important. A broad classification of problems is additionally frequently studied, ranging from relaxation behaviour of complex fluids, molecular liquids, dynamics of energy storage and battery components, and magnetic spin relaxation in correlated electron systems. A similar detailed analysis for Europe and Japan is not possible immediately (publication records are not clearly published per instrument, and the better instruments are relatively new). Choosing one year (2012) to search publications from the respective facilities places water and biomolecules as the most frequently studied, followed by polymers, electrolyte materials and complex fluids.
There currently seems to be a marked difference in the balance of problems addressed on IRIS/OSIRIS when compared with other backscattering instruments. Increasing the energy resolution of OSIRIS should open the opportunity for the instrument to address important, and elsewhere more frequently studied, problems in biomaterials, polymers and water-rich systems. In addition to the proposed upgrades, in the longer term the team might also want to consider implementation of a FIRES-type backscattering instrument. This would enhance technical performance in terms of both resolution and dynamic range, and help to further strengthen and maintain the user program.

The spatial and temporal ranges accessible using QENS are ideally matched to the atomic and molecular vibrational displacements, correlation lengths and diffusive motions encountered in highly complex biological systems. To date, one of the problems often encountered by the user community is the need to move across different facilities to perform the experiments (the use of various elastic resolutions is necessary to disentangle the plethora of motions observable in such complex systems). With the OSIRIS upgrade this research will be readily possible at ISIS. In polymer science the combination of instruments that allow QENS studies to bring a more complete understanding of multiple contributions is very important because these systems have intrinsic dynamic and spatial heterogeneities. This area seems currently rather under-utilized at ISIS. However the proposed capabilities of the OSIRIS instrument, which will allow researchers to explore a broad time scale from the picosecond to the nanosecond range with good spatial resolution, might increase the number of applications and publications in this area. In studies of water and solution dynamics, the limitations encountered by experimentalists using neutron scattering are low flux, limited resolution and dynamical range, and the intricate analysis of the data. All of these limitations will be addressed in the proposed instrument and modelling development plans. Other opportunities exist in rotational tunnelling spectroscopy (for example H₂, CH₄, -CH₃, NH₄), hyperfine interactions, low frequency excitations in glasses (e.g. aerogels & fractons) and liquids (e.g. rotons in liquid helium), and magnetic excitations. The intrinsic good inelastic resolution provided by OSIRIS and IRIS suits all these fields of research very well.

4. The Current Business Case for a QENS Activity

The business case for QENS activity rests on the wide-range of physical-chemical phenomena that are amenable to this technique. QENS is particularly well suited for probing diffusive and relaxational motions, as well as low frequency collective excitations. For this reason relevant fields include biological systems, polymers and soft matter, aqueous and complex fluids, glasses, magnetism, functional materials, ionic and proton conductors, catalysts, H-storage and other energy-related systems, and low-energy spin excitations. We have already highlighted some specific success stories in Section 4, many of which will lead naturally to further high-impact research. In addition, the recent increase in computer power means that calculation of neutron observables from time-dependent computer simulations is now feasible for many systems.

As a result of the broad-based applicability of QENS, the user community of IRIS and OSIRIS is very strong, with approximately 120 PIs of whom around 80 are based in the UK, who published approximately 130 peer reviewed publications between 2008 and 2013. This base is nurtured via regular user meetings and Newsletters.
In terms of sponsorship, approximately 40% of all proposals submitted by UK-based PIs are supported by EPSRC grants, and around 5% are involved in programme access. A number of PIs have direct links or sponsorship from industry. QENS also plays a strong role in the training of early career researchers. Over the period 2008-2013, approximately 25 PhD theses have arisen from IRIS/OSIRIS experiments.

5. Suggestions for Technical Developments or New Instrument Capabilities

In terms of their technical capabilities, there is strong overlap between the two instruments, but OSIRIS currently shows flux gains over IRIS of approximately 3 and 9 times for the PG(002) and PG(004) analyser options respectively. Proposals for instrument and software development were presented to us by member of the ISIS Molecular Spectroscopy Group, and are summarised in Figure 1 of this review. These were examined by the panel in the broader context of QENS instrumentation, and the ISIS Target Station 1 upgrade project. This project would provide a gain of a factor of 5 for the H₂ moderator, and therefore has the strong support of the panel.
Due to the higher flux compared to IRIS, OSIRIS is identified as the priority for technical upgrades. The proposed development path for OSIRIS constitutes:

- Phase-1. Study and upgrade the secondary spectrometer by installing an Si(111) analyser bank complementary to the existing PG-analysers (£0.6M).
- Phase-2. Rebuild the primary spectrometer with new chopper system and neutron guide (£3M).

**Recommendation:**

*The panel strongly endorses the immediate implementation of the OSIRIS development plan.*

Phase-1 in the upgrade path has a modest associated cost (£0.6M) and will significantly enhance the capability of OSIRIS through improvements in energy resolution, up to a factor 2.5 compared to the current PG(002).
Phase-2: integration of the new moderator with both an optimised guide and pulse-chopper system will not only deliver a much higher neutron flux to the sample, but also further improve the energy resolution. This upgrade will increase the complementarity of OSIRIS to LET and TOSCA and will likely make OSIRIS competitive with BASIS and DNA, and around an order of magnitude down from MIRACLES for the tightest resolutions. The improved elastic and inelastic energy resolution and flux are expected to strengthen enormously the science program across the different fields. Additionally, studies of the use of Si(333) are recommended, and we suggest that consideration should be given to maintaining the existing possibilities to install an option for working with polarised neutrons.

Together these developments will provide ISIS with a unique cold-neutron spectrometer, distinct from LET for example, at excellent value for money.

IRIS:

Securing the future and sustainability of IRIS calls for a different approach to that proposed for OSIRIS. We note that since 2010 both instruments have been running at approximately ¾ capacity, due to staffing issues, while ISIS itself has recently been operating reduced cycles for financial reasons. Both issues are likely to be resolved in the short- to medium-term, leading to a reduction in the instruments’ oversubscription. As noted earlier, these currently stand at IRIS 1.52 (2009-13) and OSIRIS 1.39 (2008-2013). For IRIS to be viable it is therefore essential to increase the user-base.

The proposed development path for IRIS constitutes:

- Phase-1. ‘High-throughput’ QENS.
- Phase-2. Upgrade primary and secondary spectrometer.

Recommendations:

- **Phase-1. Efforts to broaden the user-base and develop more automated sample environments and procedures should be pursued.**

  Building partly on the success of the Xpress access route, the instrument team have proposed a Phase-1 pathway to increase demand for the instrument by offering high-throughput QENS, with the aim of increasing the rate at which systems can be studied by a factor of ten. This initiative may also serve to increase activity in areas such as polymers and biomaterials. Strategies include the automation and standardisation of sample, experimental and data analysis protocols. These efforts offer excellent value for money and are transferable to OSIRIS, and potentially across ISIS. Members of the ISIS Molecular Spectroscopy team described a future for IRIS centred on making this a first port of call for potential QENS users, and extending the Xpress model more broadly and contributing to a neutron scattering of biological molecules database. This would be achieved by streamlining sample changes, temperature sweep capabilities, and data reduction protocols ensuring a less manpower intensive operation than the current system. The vision is to use this as a ‘high throughput’ operation that can scan a library of sample compositions, but the sample can also be probed using complementary techniques such as calorimetry, and spectroscopy. This process has the panel’s support, since it is low cost and is transferable across ISIS.

- **Phase-2. The panel recommends a review of the options for the beam-line once Phase-1 has had time to bed in.**
Use of IRIS as an Xpress instrument and potential new QENS user recruiting tool is an option for the management to consider. Depending on the success of this program, decisions to perform a physical upgrade for the IRIS spectrometer or open the beam-line to other uses including a potentially new FIRES type instrument should be re-considered. Considerations for upgrades include a new guide, choppers, and investigating the utility of installing Si(311) analysers or a SANS detector. Phase-2 options include upgrade of the existing instrument, or a new build on the beam-line (for example based on the FIRES or ELF proposals). Based on the information available, including over-subscription rate, instrument capabilities and potential redundancy between instruments at ISIS, we do not consider that upgrading IRIS is currently a priority. Rather, when Phase-1 has had time to bed-in, we suggest a review of the beam-line.

6. Future Needs for Data Analysis and Modelling

Notwithstanding the excellent proposal-to-publication rate for these instruments, data analysis and modelling remain significant issues, and ones that are highlighted in user questionnaires and the review documentation. The computational and support development plan constitutes:

- Data reduction and MANTID integration.
- Modelling Phase-2. Extension to other HPC initiatives.

Recommendations:

- **User friendly data reduction and analysis within MANTID should be a high priority.**
  
The introduction of MANTID has the potential to greatly improve accessibility, and integration of the QENS tool-kit within this open-source software is a priority. It should be relatively straightforward for users to perform data reduction and analysis in a streamlined environment such as MANTID.

- **Phase-1. The panel supports hardware upgrades and personnel for time-dependent modelling.**
  
The need for detailed modelling of QENS spectra is unquestionable, to allow calculation of the neutron observables from time-dependent computer simulations. With this in mind, an ambitious work plan of first-principles and force-field based calculations is proposed as a high priority. The implementation of a program to provide this service is anticipated to be complex. The breadth of science in analyzing QENS data is very broad, as seen in the scientific examples. This phase has the panel's support, though we recommend that the mechanisms for choosing systems and identifying collaborators should be discussed in detail with the ISIS management and stakeholders.

In addition, this plan will be challenging for an individual to deal with. Consequently, this implies a significant investment in hardware and personnel that would need suitable mentorship. It should be investigated if such personnel are best integrated in the QENS team, rather than in the central scientific computing group for example.
• **Phase-1. Methodologies development and further integration in to MANTID should be pursued.**

The ability for external users with their own simulations to compare calculation to experiments is valuable. *MANTID* users would benefit from other facility buy-in for the development and implementation of the wrapper-codes and inclusion of varied high-level modeling codes.

• **Phase-2. Extension to other HPC initiatives should be reviewed during Phase-1.**

Phase-2 extends to other HPC initiatives, and, we suggest, should be reviewed during Phase-1.

7. **Other developments or provision which will develop the capacity or effectiveness of IRIS/OSIRIS/QENS studies at ISIS**

IRIS, if partly freed from a user program, could be an ideal test bed for more complex and new sample environments, including *in situ, in operando* and simultaneous measurements with complementary techniques such as DSC, optical, dielectric, NMR, humidity control. Such environments should, however, be user driven to guarantee a sufficient user-base. An official ‘call for tenders’ for such new possibilities might incite user groups to get involved. Many of these tests are probably time consuming, and a busy user instrument will not be able to offer sufficient time and personnel. Developments should be sufficiently standardised to fit at least into OSIRIS (and maybe LET) after successful testing on IRIS.

8. **Any other comments the panel wish to make to the ISIS Director**

Among the other factors that have contributed to the strong scientific performance of both IRIS and OSIRIS, the panel would like to highlight the enthusiastic and knowledgeable team of beam-line scientists, particularly bearing in mind that the QENS team of the Molecular Spectroscopy Group has recently been down to 3 members of experimental staff. In addition, it is worth noting the excellence of the sample environment support at ISIS which enables technically challenging experiments to be conducted routinely.

While the suggestions for modelling support of QENS experiments are timely and well received, a general external review of the scientific computing provision across ISIS might provide a more holistic view – for example identifying common themes and opportunities across the instrument groups.