

ISIS User Committee

Friday 15 June 2012, 10:00 am

The Cosener's House, Abingdon

The User Committee represents the ISIS user community on all aspects of ISIS operations.

Committee members are drawn from ISIS user groups and ISIS senior managers.

Users may pass any comments or concerns they have about ISIS to the user group representatives or contact the Chairman of the ISIS User Committee, David Lennon.

Urgent matters are dealt with as they arrive. Less urgent matters are discussed at the next meeting of the committee. Committee meetings are held immediately after the facility access panel meetings in June and December.

IUC Membership

| | | |
|------------------------------------|---|---|
| Chairman | D Lennon | University of Glasgow |
| IUG1 Crystallography | A Powell Vacancy | Herriot Watt University |
| IUG2 Liquids & Amorphous Materials | J Holbrey B Webber | Queen's University of Belfast University of Kent |
| IUG3 Large Scale Structures | A Zarbakhsh J Lakey | Queen Mary College, London Newcastle University |
| IUG4 Excitations | J Goff P Salmon | Royal Holloway University of London University of Bath |
| IUG5 Molecular Spectroscopy | S McLain D Lennon | Oxford University University of Glasgow |
| IUG6 Muons | D Paul A Drew | Warwick University Queen Mary College, London |
| IUG7 Engineering | M Preuss D Dye | University of Manchester Imperial College London |
| U Steigenberger | Acting Director ISIS | |
| P King | Acting Division Head, ISIS Spectroscopy and Support | |
| S Langridge | Division Head, ISIS Diffraction | |
| Z A Bowden | Division Head, ISIS Experimental Operation | |
| D Greenfield | Division Head, ISIS Instrumentation | |
| A Kaye | ISIS User Programme Manager Secretary to the ISIS User Committee | |

Apologies were noted from: Z A Bowden, D Paul

Andrew Taylor, STFC Executive Director, National Laboratories, attended the meeting.
John Womersly, STFC Chief Executive, attended for item 7.
Steve Wakefield attended on behalf of the ISIS Experimental Operations Division Head.

1. WELCOME

The chairman David Lennon welcomed the IUC members.

2. MINUTES AND MATTERS ARISING

The minutes from December 2011 meeting were noted and approved.

All actions from the previous meeting were noted as complete, with two exceptions.

The chairman noted that several groups did not send in summary reports to the Secretary for inclusion in the minutes. He stressed the need to do this this time.

| | | |
|--------------------|---|--------------------|
| ACTION: 2.1 | IUC group members written reports from Groups must be sent to A Kaye within a week of this meeting. | IUC Members |
|--------------------|---|--------------------|

It was also noted that the action on U Steigenberger to feed to and from the IUC to the IOP in the new Facilities Forum was ongoing. Uschi is on the IOP Science Board.

| | | |
|--------------------|---|------------------------|
| ACTION: 2.2 | U Steigenberger to report back to the IUC about how this is progressing | U Steigenberger |
|--------------------|---|------------------------|

It was noted that this would be David Lennon's last meeting as IUC chairman and that he would also be standing down as the Molecular Spectroscopy Representative.

| | | |
|--------------------|--|---------------|
| ACTION: 2.3 | To start the process for appointing a new Molecular Spectroscopy Representative and new IUC chairman | P King |
|--------------------|--|---------------|

3. CHAIRMAN'S REPORT

The IUC were updated on staff changes within ISIS and STFC. Andrew Taylor has a new role as Executive Director for National Laboratories and is therefore no longer ISIS Director.

Uschi Steigenberger is now acting ISIS Director. The ISIS Director post has been advertised and interviews have taken place.

John Womersley is STFC CEO and he has a new team of Executive Directors of which Andrew Taylor is one for National labs. Directors representing Finance, Strategy, Business and Innovation, and Corporate Services are in place and interviews have taken place for the remaining Directorship, Programs.

The IUC congratulated Andrew Taylor for his good work. The committee wished to thank Richard Wade for his help and support.

| | | |
|--------------------|--|-----------------|
| ACTION: 3.1 | IUC Chairman to write letter of thanks to Richard Wade | D Lennon |
|--------------------|--|-----------------|

It was reported that a meeting had taken place in London as part of EPSRC's requirements capture process for the Facility Funding Model. The meeting was attended by several IUC members plus ISIS instrument scientists. The Chairman showed slides from the meeting illustrating the process being followed. The conclusions of the meeting included an

endorsement of full operations of ISIS and a need to do something about the loss of studentships. All parties will sign off on this document by August.

The next ISIS Facility Advisory Board will be on the 4th of July. The Chairman will attend this meeting, and will aim to have the EPSRC requirements document discussed.

The IUC also requested that the minutes of their meetings be made available publically.

| | | |
|--------------------|---|---------------|
| ACTION: 3.2 | IUC minutes to be made publically available on the web. | A Kaye |
|--------------------|---|---------------|

4. REPORTS FROM USER GROUPS

4.1 Crystallography

The Crystallography User Group held its annual Meeting on 3/4 November 2011 at Cosener's House Abingdon. The meeting, held jointly with the Physical Crystallography Group of the BCA and the Condensed Matter Physics Group of the IOP, attracted 65 registered participants. In addition to two invited lectures (Profs J.P Attfield and J. Goff), four contributed talks by young researchers and over twenty posters were presented. Scientific themes included: exploiting the complementarity between neutrons and other techniques; studies of hydrogenous materials, including hydrogen-bonded systems; disordered systems and archaeological investigations. Discussion at the meeting covered access mechanisms, including the collaborative R&D scheme with industry; possible involvement in an Easter meeting in collaboration with the RSC solid-state group; ISIS reliability and pre-experiment administration, including the need to repeat the ERA for rescheduled (part) experiments. Users expressed a high level of satisfaction with the suite of ISIS crystallography instruments and the quality of scientific and technical support. In the Spring of 2012 Prof. Duncan Gregory concluded his term as IUG1 representative on the User Committee. The process to identify a new IUG1 representative has been initiated.

4.2 Disordered Materials

We welcome appointment of two new instrument scientists – Dr Tristan Youngs and Dr Sam Callear. Their experience and skills in experimental and computer modelling, crystallography and advanced sample environment instrumentation will be invaluable to help enhance the 'user experience', to nurture interest using these spectrometers from the wide research community and to support the development of user community programmes in complex systems and science (gas storage materials, battery materials, nanostructured catalysts etc.).

Translating the high quality data collected on NIMROD into high impact results remains a challenge to the community. There may be many reasons, including the increased difficulties in treatment of inelastic scattering, in modelling and data handling over such wide Q-range, and in simply discovering what are the best uses for this outstanding tool. From the experimenters' perspective there are, naturally, concerns about the projected restricted operation time available over the coming year and the impact that this will have on the ability to do science. This is a possible cause of the apparently self-regulated reduction in applications of beam time from established investigators.

Feedback from users via the web interface appears to be largely very positive with general representative comments including "Excellent facility. Staff, scientific and instrument support unparalleled anywhere else", "Very good equipment, competent and friendly personnel, lots of help with data treatment", "Instrumentation is remarkable. User support is above and beyond expectation or duty." although some users (inevitably) suffered

from “Bad beam reliability”. Amongst suggestions for future provision were the development of more “inter- and intra-disciplinary meetings” and further “opportunities for [users] to interact with each other and with staff at ISIS” After some discussion, these are excellent suggestions of ways to engage users within the ISIS community rather than feeling isolated.

4.3 Large Scale Structures

The large scale facility users have expressed their appreciation of the availability of a series of dedicated sample environment for large scale structure experiments. Particular thanks go Mr Andy Church for maintaining the sample environments in Soft Matter Science.

There is a plan for a Large Scale structure meeting to be held at the Cosener’s House in September 2012.

A range of complementary characterisation techniques (AFM, XR, XRD) are now available in the Large Scale Structure Group for sample preparation/characterisation prior to neutron experiments. These are extremely well maintained and used.

Overall feedback from users was positive. The efficiency and friendliness of User office personnel and the high level of support received from instrument scientists were strongly appreciated. The laboratory facilities are much appreciated and contribute to better success particularly in biology experiments. There is a need for more accessible data treatment and fitting software and Mantid is appreciated as a step in that direction. However this is the stage in any experiment that will always be challenging for occasional users and the developments should continue.

4.4 Excitations

The IUC meeting was immediately followed by the Excitations User Group Meeting on 27 June 2012. This was scheduled to run the day before the “Theoretical & Experimental Magnetism Meeting” on 28 -29 June 2012, in an attempt to boost attendance and obtain input from overseas users. The points raised at the IUC and in the web survey were used to seed discussion in the Excitations User Group Meeting.

Rep-rate multiplication has been employed on LET in order to fill the time frame and obtain data at several incident energies. Quasi-elastic neutron scattering studies of hexadecane give $S(Q,t)$ data that overlay and cover three decades in time in one shot. It was possible to measure the full bandwidth and focus in on the energy gap in one shot for the quantum spin chain CoNb_2O_6 . The Flynn ^3He filling station is able to polarise up to 80% in 100s. The first polarised tests have been performed on LET.

New guides have been proposed for MAPS and MARI. These will give an order of magnitude increase in flux with negligible degradation in instrumental resolution. This would extend the useful energy range to smoothly crossover with LET at similar resolution, and this would enable more challenging experiments in the areas of hydrogen storage, ionic liquids and inorganic glasses. It would ensure that the flux at ISIS is comparable to SNS instruments across the whole suite in the Excitations Group. This proposal was strongly endorsed at the Excitations User Group Meeting.

The LET guide is currently optimized to give a uniform beam across a large area, so that studies can be performed on aligned arrays of crystals. It is proposed that by allowing pivoting of the guide after the chopper, it will be possible to focus the beam on the smaller samples more typically supplied by users to obtain double the intensity. Again

this proposal was supported at the Excitations User Group Meeting since it was acknowledged that it is not always possible to turn up with an array of aligned crystals.

The web survey was a useful source of feedback. Perhaps the points raised and brief responses could remain on the web site on a continuous basis, with occasional prompts for users to provide feedback?

"The main shortcoming is off-site access to data during and after the experiment. What is needed is the ability to log in remotely, process the raw files and copy them to the host institution. I believe this is possible on some instruments, but it is not widely known how one goes about getting access." It is possible to do this at present, but it usually requires intervention from an instrument scientist. It was agreed at the Excitations User Group Meeting that this is a substantial issue that ISIS will have to address.

"Allocate sufficient manpower to as quickly as possible install remaining detectors on LET." This is a top priority of the Excitations Group, but the main difficulty has been troubleshooting problems with the new detectors. Up to 50% may have to be returned to the manufacturers under warranty. However, it is anticipated that the full detector bank will be in place by the end of 2013.

"Provide a dedicated cryomagnet with integrated dilution refrigerator. The refrigerator should sit in the main isolation vacuum so only the outer wall of the cryostat and some very thin radiation shields are in the beam." This reinforces the user demand for dilution refrigeration, and indicates the need for users to have more input in facility development. Complementary funding from other research councils would be ideal, but input from users in the current process might help.

A meeting on "Dynamics in Crystalline Materials, Glasses and Soft Matter" will be held at Cosener's House from 10 -11 September 2012. This will complement the "Theoretical & Experimental Magnetism Meeting", and it will be a new source of feedback from a different area of the Excitations Group user community.

4.5 Molecular Spectroscopy

The MSUG was pleased to hear that there are 3 new positions that have been filled in the MS group at ISIS, specifically 2 which focus on data analysis/computation and one which replaces Jerry Mayer on Vesuvio. The MSUG was also pleased that Vesuvio is now back online and that this instrument has survived its potential shut down after rumours of such over the last few years.

David Lennon has now retired as both the chairman for the IUC and as the user group representative (secretary) for the Molecular Spectroscopy User Group. The MS group at ISIS will choose/appoint the next representative. Sylvia McLain will retain the post of chairperson of the MSUG.

After implementing a joint idea (of Jeremy Lakey and Sylvia McLain) for putting comments online for Users and then disseminating these to the User group chairs, the MSUG received a total of 15 comments/complaints. The feedback was in general very positive with specific mentions of ISIS User support by instrument scientists where it was universally acknowledged that this support was exceptional. Guides were requested for MARI, MAPS and TOSCA, where TOSCA guides are planned for the future by the MS group at ISIS. There were also several requests for MANTID to be implemented for data analysis on all MS group instruments, where this implementation is already under way.

4.6 Muons

A successful Muon Training School was held in March this year with 20 students in attendance. A Muon User meeting will be held in September celebrating 25 years of Muon's at ISIS and Steve Cox's retirement.

The User feedback was very positive especially when describing local contacts and sample environment support. However the vending machines and magazines in the coffee room were heavily criticised.

Users felt there was not enough beam time available.

It was also noted that Mark Telling had joined the Muon group; he brings with him his interests in the bio sciences.

4.7 Engineering

Note summarising presentation as no report yet received from IUC Member.

It was noted that although Engin-X is the primary engineering instrument, a lot of other engineering studies are going on at ISIS, specifically on SANS, GEM, HRPD and also SXD. There is an ongoing need for more resolution on Engin-X. Much of the work is on stress loading and users are requesting more engineering load rigs and furnaces. ENGIN-X is nearly 10 yrs old now.

It is good news that a new instrument scientist is starting in this group.

Concerns were generally expressed about the problems of sharing large datasets (terabytes of data) on the web.

The users need joined up reporting systems for experiments and grants. There is an urgent need for STFC and RCUK as a whole to unite the systems, as people are drowning in admin. The web based systems need to find publications and grants automatically.

A need for easy access to more pictures of ISIS was expressed to help the community in presenting the facility.

5. UPDATE ON ISIS OPERATIONS

Last year, the basic programme of 120 days on all instruments was not initially fully funded. Additional funds were provided by STFC through support for the Industrial Collaborative R&D (ICRD) scheme which is proving very successful in encouraging further industrial involvement in ISIS. In the end, 140 days were delivered to the user community.

In the current financial year, STFC will continue to support the ICRD scheme. However, a flat budget and increased costs, including utility costs, means that at present there are funds to guarantee delivery of only 95 operational days. ISIS and STFC are actively working to enable at least 120 days of operations for the year.

6. REF AND FACILITIES

ISIS has sent out bank statements to UK PIs which have been very well received. REF data has also been sent via STFC and RCUK to HEFCE, who make it available for institutional contacts on their extranet. Users can discover their REF institutional contact: see <http://www.ref.ac.uk/contact/>. It was noted that no Co-I information was provided; while

this is not a problem if Co-Is are at the same institution as the PI, if they are at different institutions then it is up to the PI and Co-I to split the award between themselves.

| | | |
|--------------------|--|---------------|
| ACTION: 6.1 | Put this REF info onto the ISIS external website and also add instructions on what to do | P King |
|--------------------|--|---------------|

7. ISIS NEUTRON TRAINING COURSE

This course was seen as a really positive contribution to the training of students. The course was heavily oversubscribed (4:1). The IUC requested more places and more clarity of the selection procedure. ISIS would like to work with the community to see how more access can be provided.

| | | |
|--------------------|--|---------------|
| ACTION: 6.2 | Raise this at the next meeting with regards to staff time and beam time. | P King |
|--------------------|--|---------------|

8. USER FEEDBACK AND FOLLOW UP

The online user feedback process had been seen as beneficial and a success: around 80 responses from the community had been received and passed to the relevant IUC representatives. The IUC asked for follow-up to be publicised to the community.

| | | |
|--------------------|---|---------------|
| ACTION: 6.2 | Summarise the issues raised, and actions and responses. | P King |
|--------------------|---|---------------|

9. IUC DISCUSSION WITH JOHN WOMERSLEY STFC CHIEF EXECUTIVE

REF: REF panel should be aware of ISIS time awarded to users. ISIS / STFC is providing this information to HEFCE (see also agenda item 6).

Studentships: The issue of studentships was discussed. A lot of facility users have been dependant on EPSRC studentships funded through grants, a mechanism which EPSRC has discontinued. Can STFC help? EPSRC and STFC together used to have a scheme called next generation facility users. STFC should consider studentships targeted at facility development; part-funding for students in collaboration with university partners would be very attractive. Users should also consider setting up DTCs based on neutrons/muons.

Public engagement funding: STFC will support a fraction of a researcher's time for outreach. There will be a call for proposals later in the year. Publicising ISIS-related work will be part of the requirements.

Facility funding: The community is concerned about the way that ISIS and CLF are funded. The Drayson model partitions STFC funding into three areas:

- Overseas subscriptions
- UK facilities
- Programmes (research grants for the particle physics and astronomy programmes)

UK facilities are Diamond/ISIS/CLF. Funding for ILL/ESRF is covered through the overseas subscription line. The RCUK budget for UK facilities is presently 5.6% of the total RCUK budget. John Womersley stated that he is committed to keeping ISIS as a world leading facility. EPSRC's programme relies on having access to facilities. The Klein report on chemistry, for instance, points out the importance of facilities like ISIS. Neutrons

underpin a very broad programme; case studies on the impact of neutron research are of high importance and cooperation from the user community is essential in preparing them.

The user community could also promote ISIS in their own talks, and material needs to be made available to help them do this.

| | | |
|--------------------|---|---------------|
| ACTION: 9.1 | Make material available on the ISIS website for users to use in promoting ISIS. | P King |
|--------------------|---|---------------|

The Chairman thanked John Womersley for his time.

10. DATE OF NEXT MEETING

The next IUC meeting will take place on Friday the 9th of December 2012. As usual it is planned that the Chairman will host a private dinner for members who arrive the evening before the meeting.

11. A O B

David Lennon was thanked by the IUC for his hard work as IUC Chair over the past three years.

APPENDIX:

ISIS Programme Update (Philip King)

Not delivered due to timing of discussions with John Womersley

- In addition to TS-2 Phase 2 instruments, a variety of other instrument developments are ongoing. These include completion of detectors on LET, refurbishment of the primary muon beamlines, Be filter for Osiris, completion of detector banks on Pearl and Wish, and development of the polarised neutron programme.
- We have just heard about an award of around €4M by the Dutch research organisation NWO for polarisation development on Larmor. Alan Drew at Queen Mary London has also just received a €1.5M grant to develop a laser system for the HiFi muon instrument.
- Mantid continues to develop as a data analysis and visualisation framework for neutrons, with several neutron sources around the world now involved. We would like to work with community members to develop analysis software within the Mantid framework.
- The ISIS Industrial Collaborative R&D scheme is proving very successful, with 67 days of instrument time already allocated since the scheme began last year.
- Recent events at ISIS have included a day celebrating ISIS' collaborative activity with Sweden, including opening of the upgraded Polaris instrument; successful training courses for post-grad and post-doc students in both neutrons and muons; and a celebration of 25 years of muons at ISIS.
- The UK Neutron and Muon User Meeting (NMUM) was held in April. We would value comments from the community on future formats of this meeting. Sylvia McLain from Oxford was awarded the Willis Neutron Scattering Prize at NMUM for her work on biological molecules.
- The Facilities User Office will be relocated to the RAL Reception building this summer. A new online Visits system will be rolled out shortly which will give new functionality for users booking visits to ISIS.
- REF data has been submitted by ISIS to RCUK (who will forward it to HEFCE). It is then up to institutions to manage/distribute this information to departments. Institutional REF representatives can be found by going to the following web page:
<http://www.ref.ac.uk/contact/>.