

ISIS User Committee

Friday 7 December 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, Jon Goff.

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 – December 2012

Chair	Jon Goff	Royal Holloway University of London
IUG1 Crystallography	Anthony Powell	Herriot Watt University
	Peter Slater	University of Birmingham
IUG2 Liquids & amorphous	John Holbrey	Queen's University of Belfast
	Beau Webber	University of Kent
IUG3 Large Scale Structures	Jeremy Lakey	Newcastle University
	Ali Zarbaksh	Queen Mary College, London
IUG4 Excitations	Jon Goff	Royal Holloway University of London
	Phil Salmon	University of Bath
IUG5 Molecular Spectroscopy	Sylvia McLain	Oxford University
	Christoph Salzmann	University College London
IUG6 Muons	Don Paul	Warwick University
	Alan Drew	Queen Mary University of London
IUG7 Engineering	David Dye	University of Manchester
	Michael Preuss	Imperial College London

Robert McGreevy	ISIS Director
Zoe Bowden	Head ISIS Experiment Operations Division
Debbie Greenfield	Head ISIS Instrumentation Division
Philip King	Head ISIS Spectroscopy and Support Division
Sean Langridge	Head ISIS Diffraction Division
Andrew Kaye	ISIS User Programme Manager
Christy Kinane	Recording Secretary

Apologies were noted from: Beau Webber, Jeremy Lakey, Phil Salmon, Alan Drew, Christoph Salzmann, David Dye, Michael Preuss and Zoe Bowden.

Steve Wakefield attended on behalf of the ISIS Experimental Operations Division Head

1. WELCOME

Jon Goff was introduced as the new Chair of the ISIS User Committee.

The Chair welcomed Robert McGreevy as new Director of ISIS.

The Chair will write a letter to thank David Lennon for his work during the tenure of his Chairmanship.

Action 12-2-01 Jon Goff to write to David Lennon **Jon Goff**

It was noted that Christoph Saltzman has replaced David Lennon as one of the molecular spectroscopy user representatives; and Peter Slater was welcomed as a new crystallography representative.

2. MINUTES AND ACTIONS ARISING

The minutes from June 2012 meeting were noted and approved. These minutes are publically available on line.

All actions from the previous meeting were noted as complete. Further follow-up actions:

Action 12-2-02 To invite Uschi Steigenberger to next IUC meeting to report on the progress of the facilities forum at the IOP **Philip King**

Action 12-2-03 Send letter to university departments to remind them where to find the REF reps information. Also send this to the PI's? **Philip King**

It was noted that it is in general difficult to get feedback from users on their experience at ISIS, and that the web consultation in advance of the IUC meeting worked well last summer. The committee decided that the consultation should be left open all the year round but that the User Office should still send out a reminder biannually.

Action 12-2-04 The User Office should open the User Feedback system and make the user community aware of it at every opportunity **Andrew Kaye**

Action 12-2-05 ISIS should make material available on the ISIS website to enable users in promoting the facility. Things like pictures, videos, logos, etc. **Philip King**

3. CHAIRMAN'S REPORT

STFC is presently engaging in its Programmatic Review. This looks at the whole STFC programme, including facilities, with the aim of informing STFC's strategic plans on the timescale of 10 years or so.

The Research Councils' Facility Funding Model process is also on-going alongside the STFC Programmatic Review. The RCs produced a requirements document for facilities, to which facilities have been asked to respond. This will result in STFC

producing an options document which will go back to the Large Facilities Steering Group to inform funding decisions. The user community have been concerned about a lack of feedback and transparency within this process.

4. Reports from User Groups – achievements and issues arising

Each user group gave a short (5 minute) report on activities.

a. Diffraction:

The Annual Meeting of the Crystallography User Group was held at Cosener's House on 8/9 November 2012. The meeting, with the theme "The Crystallography of Functional Materials", was held jointly with the Physical Crystallography Group of the British Crystallographic Association and the Structural and Condensed Matter Physics Group of the Institute of Physics. Over 80 participants attended the meeting. In addition to invited lectures (Prof. P. Slater, Drs I Abrahams and J. Claridge), four talks were given by young researchers and 22 posters were presented. Scientific themes included materials for energy applications, the exploitation of complex sample environments, framework solids, multiferroics and complex magnetic structures.

Recent developments within the Crystallography Group at ISIS were outlined. The completion of the Polaris diffractometer and the recommencement of the User program are of particular importance to this User Group. An overview was given of significant scientific results from the year, including the first paper to arise from experiments on the upgraded Polaris diffractometer, the use of Polaris to study extremely small samples, work facilitated by the GEM express service and investigations carried out by industry. The principal topic of discussion at the meeting centred on access mechanisms and in particular whether alternative mechanisms may provide more efficient use of the available beam time. In addition, users expressed a high degree of satisfaction with the suite of ISIS crystallography instruments and the quality of scientific and technical support. The meeting welcomed Prof. Peter Slater as the new IUG1 representative.

b. Disordered Materials:

There continues to be interest in using the DM instruments from a broad user community (with proposals addressing challenges in chemistry, physics, biology and materials science). With its recent updates, NIMROD now has a complete detector array enhancing both the count rate and Q-range available. On the data handling side, there have been interesting developments within the latest versions of GUDRUN to use iterative processes to treat inelastic scattering, which will hopefully help address the continuing challenge in data reduction. The User Group meeting is scheduled for February 2014 at Cosener's House and will be followed by training sessions in data reduction (GUDRUN) and simulation (EPSR).

c. Large Scale Structures:

The LSSG held their User Group meeting on 3th to 4th September 2012 at the International Space Innovation Centre, Harwell. The meeting was well attended by both PIs and research students. There were plenary lectures covering a broad area of science relevant to this community. There was a poster session followed by an

informal dinner at the ISIS Staff Club in the evening and we also had an opportunity to celebrate the iconic instruments CRISP and LOQ and the substantial contributions they have made to scientific endeavours.

The final session of the meeting covered the recent changes to the ISIS user Office. There was a talk on the update on MANTID, followed by a talk on the "ICRD scheme". Considerable appreciation was expressed for the dedicated staffing in sample environments and the subsequent improvement in all aspects of sample environments used by the LSSG. Concerns were raised regarding the staffing level of instrument responsible scientists which has resulted in a reduced scheduling of some of the instruments.

d. **Excitations and Polarised neutrons group:**

A Symposium and User Meeting on the Dynamics of Crystalline, Soft, Biological Disordered Systems was held at Cosener's House from 10 – 11th September 2012. The aim of this meeting was to discuss issues for current and potential users of the suite of spectrometers in the Excitations Group that are not covered by the User Meeting accompanying the Theoretical and Experimental Magnetism Meeting. There were scientific sessions on functional materials and soft matter with topics spanning hydrogen storage materials, catalysts, network forming glasses, thermoelectric materials, the biology of the eye, and the delivery of pharmaceuticals. A session on techniques covered both direct and indirect geometry spectrometers, and focussed on new opportunities with LET. There were scientific talks on first-principles density-functional and molecular dynamics simulations, and there were talks on C-lab at ILL and the Mantid project. The operation of the industrial collaboration at ISIS was reviewed.

The user discussion focussed mainly on the need for density-functional and molecular-dynamics simulations to understand the neutron spectra. This is true for the simplest case of phonons from single crystals, and it is a prerequisite for most studies of the dynamics of more complicated biological systems. Increased support for high-end computing would allow better analysis of current data sets, providing a route to higher impact publications. Better support for neutron users would lower the barrier to new users, particularly in the area of the dynamics of biological systems. There would seem to be an opportunity to build on the experience of the C-lab at ILL, and to draw on world-leading experience in the Scientific Computing Department at STFC, to establish a substantial activity in this area at ISIS.

There are clearly new opportunities with rep-rate multiplication on LET. However, for quasi-elastic studies, it is not yet clear to users how LET compares and complements the indirect geometry spectrometers at ISIS. The users at this meeting supported their colleagues in the magnetic excitation community in requesting that the provision of the full bank of detectors to high angle should be the number one priority. It was identified by users that collimation is necessary to suppress a large and complicated background from cryofurnaces for quasi-elastic measurements, and polarisation analysis would be useful in isolating incoherent scattering.

e. **Molecular Spectroscopy:**

The MSUG successfully held a successful two day science meeting on 14-16 November 2013 at Cosener's House, which marked the occasion of the retirements of Dr. John Tomkinson and Dr. Jerry Mayers.

The meeting was well attended by many ISIS Users both from the UK and abroad, with a total of over 80 attendees. The meeting was split in five sessions covering the breadth of the MSUG. The broad range of topics covered in this user group were energy and environment, catalysis, quantum systems, soft matter & biology, and theory & modeling as well as a session for a user group discussion, led by the MSUG chairperson, Sylvia McLain

The MSUG has also chosen a new representative, Dr Christoph G Salzmann from the Department of Chemistry, University College London upon the retirement from this post of David Lennon (Department of Chemistry, University of Glasgow). the MSUG thanks Dr. Lennon for his service and welcomes Christoph Salzmann to this new post.

f. **Muons:**

- Frontiers in Muon Spectroscopy meeting held in September in Oxford, partly to mark the retirement of Steve Cox.
- Science continues to focus on superconductivity and frustrated magnetism, but with muoniated radical chemistry also developing.
- Alan Drew has been awarded an EU grant for new Laser on HiFi to develop pump-probe experiments.
- Recent work on muon data acquisition systems has led to count rate improvements on MuSR which will be rolled out to other instruments in the near future.
- New Dilution fridge for the muon instruments and a new power supply for the Emu main magnet are going ahead.
- Staffing: Adrian hillier has taken over a group leader and a new PDRA Jamie Peck has been appointed on an EU grant. Sean Giblin has moved to Cardiff university.

g. **Engineering:**

Joe Kelleher gave a short overview of developments in the engineering section.

Action 12-2-06 Group Representatives to send a summary reports to Andrew Kaye as soon as possible.	IUC Members
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5. Update from the ISIS Director

ISIS should be known for excellent science and for showing leadership within its areas of operation.

The ISIS science quality remains high, as recognised by the ISIS Facility Board, and we have been able to maintain the same quantity of outputs, even though we have fewer operational days at present.

Values and concerns for the future

- Maintaining excellence (quality not just quantity) of ISIS outputs

- Time to market (at present 6-9 months between proposal and experiment and 2 years to a paper. These timescales are too long for some communities who may use ISIS in the future)
- Exploiting data (enabling better use of the data taken at ISIS)
- Synergy (with Diamond, the Research Complex, etc.)

We need to explore new ways of reducing time to market, e.g. one proposal for multiple instruments? New access mechanisms? Improving turnaround time; making better use of the data we produce.

ISIS accelerator availability is of concern, but no accelerator-based source will ever have an availability of more than around 90%. We need to better understand how down-time affects different sorts of experiments. We need to plan experiments – from amount of time scheduled to how they are run – assuming 80-90% availability so that we maximise the science output.

The ISIS equipment 'family':

- Young RFQ
- Elderly linac
- Mature Synchrotron
- Mature TS1
- Young TS2

TS2 has demonstrated that enhanced neutronic performance is not just about more proton flux or power. It is therefore not clear that an ISIS MW upgrade is the right future path for the facility in the long-term. The future upgrade path being envisaged at the moment:

- TS1 target/moderator upgrades to produce neutron flux gains across the TS1 instruments.
- Linac tanks 1, 4 Replacements to ensure continuing operation of the Linac
- Possible Linac upgrade to provide additional current to feed the synchrotron
- ISIS-2 (the next significant upgrade or renewal of the whole facility)

Robert noted that he is hoping to have an external (international) review of ISIS over the coming year. Internationally, ESS is likely to be a future reality and the UK needs a neutron strategy to determine how it wishes to engage.

6. Update on ISIS operations:

- 79 days delivered over 3 cycles so far in the 2012/13 year.
- There are now improved biolab facilities in TS2 building.
- Both Prep labs in TS1 building have been upgraded.
- TS-2 Phase 2 instruments: Chipir, Larmor and Imat builds are continuing. Zoom construction is presently delayed.
- There will be a 6-month shut-down from August 2014 – early 2015 for significant work on the TS1 extracted proton beamline and refurbishment of the muon beamline front end.

7. Neutron and Muon Users meetings 2013

8-9th of April 2013, Warwick conference centre.

8. ISIS Studentships

Sean Langridge introduced this.

Ideas are being developed for an ISIS student programme of some form. ISIS already supports a number of students in a variety of ways. We would like to develop this further, with students being more coherently supported and trained, in partnership with the community. We are looking at a model of 50:50 co-funding with universities

EPSRC will launch a call for new Centres for Doctoral Training in early 2013; the ISIS scheme should be complementary to this. ISIS studentships will need to have a facility development aspect. ISIS will also pursue partnerships within CDT applications.

The User Committee expressed support for a 50:50 student funding model.

8. AoB

USER office will relocate to the RAL reception building just after Christmas.

Date of next IUC meeting is the 7th of June 2013.