

# ISIS User Committee

Friday 8 December 2023, 10:00 – 13.00

STFC The Cosener's House, Abingdon, UK

## Minutes

### Attendance

<i>User group</i>	<i>IUC member</i>	<i>Institution</i>	<i>Attendance</i>
IUG1 Crystallography	Matthew Cliffe	University of Nottingham	In attendance
	Karen Johnston	University of Durham	In attendance
IUG2 Disordered Materials	Gosia Swadzba-Kwasny	Queens University Belfast	In attendance
	Helen Fraser	The Open University	In attendance
IUG4 Excitations	David Boldrin	University of Glasgow	Apologies
	Chris Stock	University Edinburgh	In attendance
IUG5 Molecular Spectroscopy	Alexander O'Malley	University of Bath	In attendance
	Maria Paula Marques	University of Coimbra	In attendance
IUG6 Muons	Joseph Wright	University of East Anglia	In attendance
	Ravi Singh	Indian Institute of Scientific Education and Research, Bhopal	In attendance
IUG7 Engineering	Richard Moat	The Open University	In attendance
	Mahmoud Mostafavi	University of Bristol	Apologies
IUG8 Small Angle Scattering	Wuge Briscoe	University of Bristol	In attendance
	Steven Parnell	TU Delft	In attendance
IUG9 Reflectometry	Richard Campbell	University of Manchester	In attendance
	Tom Arnold	ESS	In attendance
IUG10 Chip Irradiation	Matteo Cecchetto	CERN	In attendance (via Zoom)
IUG11 Cultural Heritage	Francesco Grazzi	CNR	In attendance

### ISIS Representatives present

Roger Eccleston	ISIS Director
Steve Wakefield	Head of ISIS Operations & Deputy Director
Philip King	ISIS Associate Director for Partnerships & Programmes
Sean Langridge	ISIS Associate Director for Science
Marek Jura	ISIS Experimental Operations Division Head
Hannah Griffin	ISIS Computing Division Head
Emma Gozzard	ISIS User Programme Manager
Ludmila Mee	ISIS BioLab Manager and Sustainability Representative

Apologies from Matt North (ISIS Instrumentation Division Head)

## 1. Welcome and introductions

The attendees were welcomed by the Chair and introduced themselves.

## 2. Minutes and matters arising

The minutes from the meeting of 9 June 2023 were approved.

### Actions from the meeting of 9 June with status comments:

Action	Responsible	Meeting action added	Update
Consider relaunching user twinning scheme (including data analysis)	Philip / Emma	Dec 2020	Ongoing
User charter – to be modified following IUC comments	Philip	June 2023	Done. Changes have been made following the last IUC meeting; Charter has been presented to ISIS Instrument scientists and further comments received. IUC has a revised version for any further comments.
Promote IUC and generic email address through post cards / posters in cabins, etc.	Emma	June 2023	Ongoing.
Experimental reports – revised form and process <ul style="list-style-type: none"> <li>Reminders to expt team (students) as well as supervisors to be explored.</li> <li>Online form to be created.</li> <li>Expose submission rates to panels.</li> <li>Additional reminder emails from Philip.</li> <li>In-kind beam fee to be withheld until report submitted.</li> <li>Guidance on report usage and reasons for collecting reports to be made more prominent</li> <li>Change report sending to last day of experiment</li> </ul>	Emma Emma Emma / Philip Emma Emma	Dec 2022    Dec 2023	Ongoing.  Difficult to do in an automated way Philip to finalise objective of expt reports Starting Dec 2023 FAPs Philip to finalise objective of expt reports  Philip to finalise objective of expt reports  New action
Students as PIs on proposals – flag for which Co-I is the supervisor and copy into correspondence	Emma		Done. Difficult to do in an automated way
Online form for notifying ISIS of publications and PhD theses	Emma		Ongoing.
DOI for multiple datasets / raw and reduced data	Hannah	Dec 2022	Ongoing – work within the New Data project.
IDAaaS information on the ISIS website and provision of computing information in general	Hannah	Dec 2022 and raised again June 2023	Ongoing – user area to be updated.
Videos on data analysis	Hannah	Dec 2022	Ongoing.
Video on Data Gateway	Hannah	Dec 2022	Ongoing.
User meetings: ensure all groups have these	Sean	June 2023	Almost all groups have had user meetings this year. Reflectometry is being explored.
User meeting list: put on web	Philip	June 2023	Done. Will go into the 2024 ISIS events calendar. Science roadshow events are already online: <a href="https://www.isis.stfc.ac.uk/Pages/science_roadshows.aspx">https://www.isis.stfc.ac.uk/Pages/science_roadshows.aspx</a>
User meeting list: periodic email to users to publicise	Emma	June 2023	Done.
Consider industrial involvement with NMSUM – Philip to discuss with Graham / Chris	Philip	June 2023	Done. Discussed with Chris. General view is not to have a separate industry event or session, but to ensure industry work is presented in the science sessions.
Is per-diem sufficient	Emma	June 2023	Ongoing. Discussions had with Facility senior staff. To monitor user spend.
Can users put money on their visitor cards?	Emma	June 2023	Done. Only on the “new style” cards

Do Ridgeway machines take user cards / credit cards?	Emma	June 2023	Done. Yes – credit cards
Issue of gas-panel training – could this be annual; can it be done more efficiently so beamtime isn't wasted?	Marek	June 2023	Done. The pressure and furnace team currently provide training for new users at the start of each experiment. Users returning within a year do not require a full retrain and will receive a shorter hand over chat at the start of the experiment. The team are also able to provide full training out of cycle, for experimental team members who can come to site during this period, which would allow them to get going with their experiment a little sooner. This may not be widely known, so we are looking at advertising this option more widely.
Onsite mass spec access?	Marek	June 2023	Done. Within the Lab support group, we are able to offer LC-MS, GC-MS and direct injection MS system within the ISIS labs. If the facilities do not meet the specific requirement the labs group can facilitate access to other departments on the campus such as DLS and RCaH.
Access to DLS and RFI kit?	Marek	June 2023	Done. The lab group can facilitate access on the user's behalf. From experience access to DLS labs has been easier.
Ease of access to RCaH	Emma to pursue; Maria Paula to send Emma an example	June 2023	Ongoing. Actually becoming harder and we are pursuing this with RCaH.
Lack of onsite accommodation at times – what is happening re Ridgeway extension?	Steve W	June 2023	Ridgeway expansion is currently not a priority for RAL Estates. The business case needs to be made. New action: ISIS to solicit user stories of how this affects experiments to make the business case and to work with Diamond on this.
Email sample shipping advice to the community	Emma	June 2023	Done. Also webpage of info linked from user webpages
Remind instrument scientists to award back sufficient time so that incomplete experiments, resulting from an ISIS failure can be completed	Sean	June 2023	Done.

In the discussion on the per-diem for UK users, the issue of the per-diem for Italian users was raised as this has not increased for many years. **Action:** Philip to raise this with Carla Andreani.

The issue was raised of whether user's RAL cards can be used in Ridgeway machines. **Action:** Emma to check.

There was discussion regarding a possible expansion of Ridgeway House to avoid users needing to stay offsite. Cases are needed showing the issues that this produces. IUC members are asked to send examples to Philip; ISIS will also solicit examples from the wider community. **Action:** IUC members and Emma.

In discussion on NMSUM, it was noted that UK undergraduates would be welcome to attend if this was thought beneficial for them.

### 3. ISIS update

- Target station 1 update: now operational with the exception of the H-moderator – this will be replaced in January.
- ISIS running: Cycle 23/2 – good operational cycle. Cycle 23/3 (October 2023) had a lot of reliability issues, and there have been further problems in the current run cycle. We are continually working on reliability to improve this.
- Latest proposal round – 738 proposals + 19 through the Canadian route – very high, with 94 unique new PIs. FAPs have just taken place.

- ISIS has received awards from the International Science Partnerships Fund (ISPF) to work with Brazil, Canada, Malaysia, Indonesia and Switzerland, providing new opportunities to encourage neutron and muon use from these countries.
- Mohamed Aouane – an ILL PhD student, now an ISIS instrument scientist – won the French Neutron Scattering Society thesis prize.
- Science highlights: hydrogels work on HIV drug delivery; carbon capture materials; thermoelectric materials; photovoltaic material charge carrier lifetime measurement.
- Instrument development plans have been created by each science group to map out future desired developments in the medium to long term. These will allow prioritisation of projects and the setting out a post-Endeavour (Endeavour-2) programme for large instrument developments.
- A year of events to mark 40 years of neutrons at ISIS will start from December 2023, including science roadshow meetings in Belfast, London, Edinburgh, Manchester and Cardiff.

There was a question about instrument lost time and the large fraction of this that was due to chopper issues. It was noted that this was largely due to a chopper failure on Merlin which caused the loss of much of the last cycle.

#### 4. ISIS Sustainability Network (ISN)

Lumilla Mee presented the ISIS Sustainability Network – a group of staff looking at how ISIS can put in place measures to improve its energy sustainability. There was encouragement of users to join the network and attend meetings so that there could be 2-way communication with the user community to share ideas and good practice. ISN will showcase what the group is doing at NMSUM. There is an opportunity for users to become sustainability champions for ISIS. Suggestions from users on sustainable ways to deal with waste generated during experiments, or sustainable disposal of equipment, would be welcomed.

**Action:** ISIS to promote the ISN in a future communication to the user community (Emma).

The topic provoked discussion regarding shipping of chemicals to ISIS.

**Action:** Marek to check shipping instructions for users needing to buy chemicals for ISIS experiments – either direct shipping to ISIS or ISIS buying on behalf of users.

There was discussion regarding local transport to / from site and the need to improve this. This issue is of concern to the wider campus, and the campus joint venture partner is in discussion with local bus companies on how transport to site can be improved.

#### 5. ISIS carers policy

A proposed policy was presented whereby ISIS will support additional caring costs incurred by users in attending ISIS meetings (user meetings, IUC, FAPs, etc).

The policy was supported by the IUC as a welcomed development to support those with caring responsibilities. There was discussion regarding support during ISIS beamtime; ISIS will keep this under review, but doesn't plan to widen support beyond meetings at present. ISIS will support additional travel costs if users need to return home during an experiment.

It was raised by IUC members that most claims may not have a receipt or invoice. This needs to be considered as part of the policy document.

It was noted that organising meetings during school term time can make it easier for those with children to attend.

#### 6. ISIS and the use of AI in proposals

A proposed policy was presented regarding the use of generative AI tools within the creation of ISIS proposals. The policy recommends allowing use of such tools as long as there is a citation or reference to show that a tool has been used.

The IUC were generally supportive of this policy. There were questions regarding how the information (that a proposal had been created using an AI tool) would be used; at the moment, there are not plans for this information to be used – rather, the citing of the use is considered to be good ethical practice.

It was pointed out that similar considerations should apply to the creation of experiment reports.

**Action:** Philip to add experiment reports to the policy.

It was noted that figure creation, as well as text, should be included in the policy.

**Action:** Philip.

It may be interesting to track success rates of proposals that have / have not used an AI tool.

## 7. Undergraduates and student update

IUC were given an update on the ISIS programme to support students using overseas facilities for neutron / muon experiments during the extended period when neutron / muon availability at ISIS has been reduced due to the long shutdown. 49 requests have been supported from 32 individual students. IUC welcomed the programme and several members expressed how useful it had been. The programme will be closing for new requests on 31 March 2024 once ISIS is back at full operating levels.

ISIS has recently introduced the ability for UK users to bring undergraduates / Masters students to experiments. This was warmly welcomed by IUC.

## 8. Discussion of user feedback and user group comments

A survey was sent to the user community prior to the IUC meeting asking specific questions related to use of the proposal system, IDAaaS and the studentship scheme as well as any general comments on recent experiences at the facility. Around 50 responses were received, and user group representatives commented on these together with any other points they wanted to raise regarding ISIS operations.

### Crystallography

- A request was made for the online safety information to be available (as a pdf file, for example) outside of the online system. **Action:** Marek to explore this.
- A recent user meeting – joint with the Physical Crystallography Group of the BCA and the IoP had attracted 160 people. The event is currently being planned for next year to include the Chemical Crystallography Group.
- One group had noted an 18 month delay in scheduling an experiment. Specific details of this to be passed to ISIS to enable follow-up. **Action:** IUG1 Matthew / Karen.

### Disordered Materials

- Many of the questions in the survey had been prompted by the DM user reps in response to issues raised by community members.
- There was discussion regarding experiment reports, and the idea raised of enabling these to be done on the final day of an experiment whilst users were still at ISIS. **Action:** Philip / Emma to explore this.

### Excitations

- Computing for data analysis was felt to have improved a lot over recent years, including remote access.
- Support from the sample environment team which enabled experiments unique to ISIS to be performed was much appreciated.

- New proposal submission system – there was discussion regarding the ability to add co-Is without them needing to create an ISIS account, but the need to have a user add their own email address to our systems means account creation will need to be maintained.
- There was discussion regarding the tension between a user needing to confirm the availability of samples at proposal time alongside the expense of creating samples without guaranteed beamtime. The best solution to this is users discussing their sample availability with ISIS scientists in advance of proposal submission. Wording of the question within the proposal system on sample availability to be checked so that it allows users to confirm the mechanism of sample production if the sample isn't currently available. **Action:** Emma.

### Molecular Spectroscopy

- There were generally good comments regarding the proposal system and studentship application process.
- There was a request to enable more samples to be added to proposals.
- IDAaaS – found to be working well with good addition of new software.
- There was concern regarding ISIS reliability and the continued issues with H-moderator which particularly affect IRIS and Osiris, but the support for students visiting other sources was appreciated.
- It was felt that the price of Ridgeway House for non-UK users is becoming an issue, possibly prohibitively for some users. **Action:** of Alex to request affected users to raise the issue directly with Philip to give evidence for this effect.
- The issue of support for molecular dynamics modelling was raised, as it was becoming increasingly needed but was hard to navigate.
- The issue of personnel to support the materials characterisation lab was raised.
- There were 82 participants at the recent Mol Spec user meeting.
- There was disappointment with the lack of progress regarding instrument upgrades for the Mol Spec community, and a request for the Iris guide to be upgraded alongside Osiris.
- The community were very enthusiastic about the proposed Sherpa polarised QENS instrument.
- The ISIS bio labs were felt to be crucial and were much appreciated, providing a capability not available at other facilities.
- The issue of data curation was raised – whether users know that data is made available after 3 years, and what is actually made available at this point. **Action:** Hannah to check whether it's just the actual data, or full log files of temperature or other instrument parameters.

### Muons

- A recent user meeting had been well attended.
- Succession planning for beamline scientists is appreciated, along with support for negative muon elemental analysis.

### Engineering

- A 20 year birthday meeting for Engin-X had been held recently.
- Furniture replacement in the Engin-X cabin was appreciated.
- Concern was expressed regarding the long lead-time for neutron experiments which might be causing some PhD students to use lab-based techniques in preference to neutrons.

### SANS

- The issue of lack of labelling of allergens in the restaurant was raised. **Action:** Emma to raise this, as it is unacceptable that users or staff need to have public conversations about their dietary needs.

- Lack of shampoo in Ridgeway was noted.
- It was reported that incorrect invoices for overseas users were being issued by Ridgeway. **Action:** Emma to explore.

### Reflectometry

- Is Ridgeway check-in before 2pm available? **Action:** Emma to check.
- Beam outages were raised as an issue, especially for kinetic experiments. ISIS will allocate additional time to such experiments to try to ensure their completion.
- There was a request for clearer information on longer ISIS downtimes.
- A specific issue was raised of an industrial user unable to complete a grant because of delays in beamtime. **Action:** Richard to encourage the user to contact Philip so that this can be pursued.

### Chiplr

- Comments generally good.
- There was a request to move the student deadline to 10 Sept to enable university sign-off after summer breaks.

### Archaeometry

- There was a request for greater explanation of what is required in proposals for archaeometry users. **Action:** Emma to explore.
- The issue of sample transport and storage for cultural heritage objects was noted.
- The overall growth of the cultural heritage area at ISIS was seen as very positive.

There was a final comment on the difficulties and associated costs of sample transport for toxic / dangerous chemicals to / from ISIS, and a request for whether such costs could be part of the consumables budget for experiments. **Action:** Philip / Marek to consider this.

## 9. AoB, Date of next meeting

Alex O'Malley was thanked for his work on the committee over the past 5 years.

Date of the next meeting: 7<sup>th</sup> June 2024.

### Actions from the meeting

Action	Responsible	Meeting action added
Consider relaunching user twinning scheme (including data analysis)	Philip / Emma	Dec 2020
Promote IUC and generic email address through post cards / posters in cabins, etc.	Emma	June 2023
Experimental reports – revised form and process	Philip	Dec 2022
Online form for notifying ISIS of publications and PhD theses	Emma	Dec 2022
DOI for multiple datasets / raw and reduced data	Hannah	Dec 2022
IDAaaS information on the ISIS website and provision of computing information in general	Hannah	Dec 2022 and raised again June 2023
Videos on data analysis	Hannah	Dec 2022
Video on Data Gateway	Hannah	Dec 2022
Is per-diem sufficient	Emma	June 2023
Ease of access to RCaH	Emma	June 2023
Ridgeway extension: ISIS to solicit user stories of how this affects experiments to make the business case and to work with Diamond on this. IUC members to send any examples to Philip.	Emma All IUC members	Dec 2023
Italian experiment support amount to be raised with Carla Andreani	Philip	Dec 2023
Use of user cards in Ridgeway House vending machines	Emma	Dec 2023
ISIS to promote the ISN in a future communication to the user community	Emma	Dec 2023

Marek to check shipping instructions for users needing to buy chemicals for ISIS experiments	Marek	Dec 2023
Policy on use of AI tools: experimental reports to be added; a note on figures to be added	Philip	Dec 2023
Online safety test material to be available as a pdf	Marek	Dec 2023
Specific example of long experiment delay to be given to Philip if possible	Matthew / Karen (IUG1)	Dec 2023
Proposal system wording around sample provision to be checked	Emma	Dec 2023
Gather evidence of Ridgeway costs prohibiting overseas user coming to ISIS	IUG5 Alex / Philip	Dec 2023
What is included in data files when data is made public to be clarified	Hannah	Dec 2023
Ridgeway invoices for overseas users to be checked for accuracy and clarity	Emma	Dec 2023
Labelling of food for allergens in R22 – strong need for this	Emma	Dec 2023
Ridgeway check-in time to be checked	Emma	Dec 2023
Greater explanation of what is required in proposals for archaeometry users	Emma	Dec 2023
Transport costs for dangerous samples – can this be part of the consumables budget?	Marek	Dec 2023