

ISIS User Committee Minutes

Friday 9 December 2022, 10:00 – 13.00

The Cosener's House, Abingdon and via Zoom

Present

<i>Committee Chair</i>	<i>Emma Barney</i>
IUG1 Crystallography	Michael Hayward (Oxford)
IUG2 Liquids & amorphous	Emma Barney (Nottingham) Gosia Swadzba-Kwasny (Queens University Belfast)
IUG4 Excitations	David Boldrin (Glasgow)
IUG5 Molecular Spectroscopy	Alexander O'Malley (Bath) Maria Paula Marques (Coimbra, Portugal)
IUG6 Muons	Joseph Wright (UEA)
IUG8 SANS	Wuge Briscoe (Bristol) Steve Parnell (Delft, The Netherlands)
IUG9 Reflectometry	Richard Campbell (Manchester) Tom Arnold (ESS, Sweden)

For item 4

Ross Stewart (ISIS, IoP/RSC NSG Chair)

For item 4

Dave Barlow (Manchester, UK ENSA Representative)

Present from ISIS:

Roger Eccleston	ISIS Director
Steve Wakefield	Deputy Director & Head of ISIS Operations
Emma Gozzard	ISIS User Programme Manager
Hannah Griffin	ISIS Computing Division Head (from 11.00)
Philip King	ISIS Spectroscopy and Support Division Head
Sean Langridge	ISIS Diffraction Division Head
Matt North	ISIS Instrumentation Division Head
Marek Jura	ISIS Experimental Operations Division Head
Sonia Conway	ISIS Business Systems
Louise Davies	STFC Scientific Computing

Apologies:

IUG1 Crystallography	Karen Johnston (Durham)
IUG4 Excitations	Christ Stock (Edinburgh)
IUG6 Muons	Lucy Clark (Liverpool)
IUG7 Engineering	Mahmoud Mostafavi (Bristol) Richard Moat (Open University)

1. Welcome and introductions

Those present introduced themselves.

2. Minutes and actions

The previous minutes were approved by the Committee

Actions from the previous meeting with comments:

Action	Status	Responsible	Meeting action added
IUC to be given a chance to comment on the 'data gateway' during its development.	Completed – presentation at this meeting	Hannah Griffin	Dec 2019
Consider relaunching user twinning scheme (including data analysis)	Ongoing – will be done once TS1 is operational	Philip / Emma G	Dec 2020
Add a page to the ISIS website on data management good practice.	Will be done in January.	Philip	June 2022
ISIS to progress User Charter	Ongoing	Philip / Emma G	Jan 2022
Crew to be asked to give updates on ISIS status at stated times	Completed – discussed at crew away day.	Steve W	June 2022
Sample can issue to be looked into	Completed	Steve W	June 2022
Can users know what evening meals will be at lunchtime	Ongoing	Emma G	June 2022
Vending machine stocking at weekends	Completed	Emma G	June 2022
Advice on methods of large file transfer	Examples of the issue are needed. We have OneDrive & SharePoint available, but if its experimental data, maybe access via the data gateway would be a better option?	Hannah	June 2022
Explore videoing of training courses	Completed – no videoing at present	Philip	June 2022
Eduroam signal in experimental halls	Completed. Facilities IT have been investigating this (working with instrument scientists) and believe we now have good coverage everywhere in the halls. If there are any further issues raised, please can we get specific examples.	Hannah	June 2022
Relaxation of 3-person limit for experiments	Completed.	Emma G	June 2022
Is further publicity for IDaaS needed?	Completed. A PM from ICD will meet quarterly and see if there are any updates/news from IDaaS for the user community and will update the website accordingly.	Hannah	June 2022
IUC visibility at NMSUM and NSG visibility	Completed. Discussion this meeting.	Philip	June 2022
User meeting calendar	Completed.	Emma G	June 2022
Generic user group email addresses	Ongoing.	Emma G	June 2022
IUC Sharepoint site	Completed.	Emma G	June 2022

3. ISIS Update

Roger Eccleston and Marek Jura gave the ISIS update, which included:

- Facility Access Panel meetings took place this week – 725 proposals were reviewed, the 3rd highest ever. There were 66 new PIs from UK and elsewhere.

- The ISIS strategy continues to be developed, with active discussions around the science strategy, and with strategies for communications, international and industrial in place and being reviewed.
- Instrument development plans are being created for the short-, medium- and long-term – with the aim of developing a long-term reference instrument suite.
- Recent operations were described for the past 3 cycles, including reliability issues in the Sept/Oct 2022 cycle.
- Deuterium lab recovery – installation of new equipment is currently taking place, aiming for start of operations next year. The deuterium team have continued to support users from a temporary lab, and a summary of recent activity was given.
- TS1 refurbishment project – the first (low power) beam to target has been achieved; beam tuning has progressed; the new cryogenic moderator systems are being commissioned. We hope to have higher power beam over the next few days, ready to run a full TS1 cycle in February.
- Facility development studentship programme: the latest call has just been completed with 9 studentships supported including 2 joint with Diamond
- Student travel support: support for students to travel for neutron or muon beamtime at overseas facilities whilst TS1 has been offline is currently in place with 28 projects supported to-date – this scheme will likely be ended once TS1 is running again.
- The Endeavour Programme – provision of 9 new instruments or significant instrument upgrades – is on track through the formal review and assurance process for funding to begin in the 23/24 year.

4. IUC and NMSUM, IoP/RSC NSG, ENSA

The summary paper noted the roles of the IUC, the IoP/RSC Neutron Scattering Group (NSG) and the UK ENSA rep in representing to the user community. The NSG had been involved in the organisation of NMSUM in 2022 and will be further involved in the 2023 meeting.

The NSG would like increased interaction with user community and will launch a survey of members in the new year to enable a SWOT-type analysis of UK neutron scattering. This will be brought to NMSUM. The ideas of getting IUC reps involved in this process was discussed, including IUC reps helping to facilitate discussions at NMSUM.

ENSA is focused primarily on European issues. Its biggest recent activity had been a consultation with users across Europe to establish current and future needs. The UK community had been contacted via the NSG, but there was a low response.

A variety of ideas for NMSUM was discussed:

- Enabling feedback from the community throughout the meeting rather than just in the big meeting on the final morning
- Using the poster session to enable feedback – e.g. IUC and NSG reps available for discussions
- Publicising what the IUC does and what it has achieved through the poster session
- Having a poster to publicise ENSA
- IUC reps available at the science day discussion sessions
- Putting the facility updates on the morning of the second (science) day so that there is time for the community to consider questions

Action: Philip, Ross, Dave to action the above list when planning NMSUM.

5. Changes to ISIS processes

- **Experimental reports:** consensus that they should be used for accountability of beamtime allocations. A more focused set of questions to be developed, and submission rates to be increased.

Action: Philip to revise the form, and look at options for increasing submission rates.

- **ORCID:** most users will have and ORCID as journals are increasingly requiring this. We should aim to capture ORCIDs, and develop methods for enabling push and pull of information to/from ORCID accounts.

Action: Emma to pursue this with business systems team

Programme access for regular users: generally not thought to be a good idea. Proposals are not that onerous, and it could lead to less efficient use of beamtime.

- **BAGS** (beamtime allocation groups) – good for Diamond as experiments can be extremely short, but not thought to be of use for ISIS beamtime.
- **Students as PIs on proposals:** Allowed at Diamond and elsewhere. Generally thought to be a good opportunity for students as long as ISIS was willing to allow students to be accountable for an experiment.

Action: Emma to check whether Diamond has had any problems, and, assuming not, enact the ability for students to be PIs.

6. User data gateway

The Data Gateway was presented as a replacement for TopCat – user access to the ISIS data catalogue – with a demonstration of its functionality.

In discussion:

- The ability to have a DOI for multiple data sets or for raw and reduced data was raised. This needs further exploration.

Action: Hannah to explore this further.

- There was discussion on how users access data: some will take reduced data away with them when they leave; increasingly, IDaaaS is being used. The Data Gateway has the benefit of being a publicly-accessible portal to ISIS data.
- There was discussion around awareness of IDaaaS and the need for further training. There is a need for further information on IDaaaS, and data analysis in general, on the ISIS website.

Action: Hannah to look at IDaaaS information on the ISIS website and a more general look at provision of computing information on the website.

- The idea of videos showing how to analyse data was discussed.

Action: Philip and Hannah to discuss this and perhaps involve the Comms team in video production.

Action: Hannah to consider a short video showing Data Gateway use and functionality.

7. Comments and reports from the user groups.

Crystallography

Many very positive comments regarding ISIS support. Higher resolution camera for tomography is desirable. Data processing could be a bit faster. Overseas length of stay – some users would like longer to analyse data. A map of site given to users when they arrive.

Action: Emma – site map to go onto the ISIS website.

Disordered materials

Vegan options (esp in Zoom café) would be good. More support is needed for data analysis. PIs could apply for a post-doc focused on data analysis; or ISIS to employ data analysis staff.

Excitations

Very positive comments esp. praising staff, and data analysis integration. Cosier cabins are needed in TS1. There was a comment about security staff friendliness when a Phd student needed to get on site at a weekend.

Molecular Spectroscopy

Like the new proposal system, but need to be able to add more than 3 samples. Access to older proposals is needed. A question was raised about reproducibility of data following instrument upgrades, and the calibration

rig for post-TS1 refurbishment was noted. There was a desire for more soft matter characterisation equipment. IDaaS was seen to work well; software issues are sorted quickly. Consistency of message regarding TS1 progress was raised – the need for more centralised communication to users.

Muons

Comments positive on support. Staff resource – negative muon support – community would support an extra instrument scientist, noting that there is only a single person involved in this area.

Engineering

No reps were present. Positive comments about staff. Public transport to/from Heathrow could be improved. More support for understanding data needed.

SANS

Very international users. Strong praise for beamline scientists; very positive comments on lab support. Downtime is a consistent issue across groups. Data reduction help needed. Data analysis support also needed.

Reflectometry

Positive comments about instrument scientist and user office support. Good range of SE kit around, but couldn't see a clear list or how to access before / after expts. Could students come for longer. Access to biolab and its kit was discussed. Alignment slow – could be automated. Inter – step into blockhouse is awkward and blockhouse needs better lighting. Carrying things into / out of lab. Lab exit is being reviewed. Vending machines only taking cash. SE well-supported, but becoming more complicated and needs more resource.

Action: Marek: look at web information on sample environment equipment and access

Action: Marek to report back on access to biolab and equipment.

Action: Marek to look at Inter step and blockhouse lighting.

8. AOB

The [BBSRC-STFC facility access funding scheme](#) was noted.

Colloid conference to be held in UK. Sarah Rogers will be the joint colloids community chair – special session on scattering; there will be a student training session, possibly with visits to RAL.

This was Emma Barney's last meeting as Chair. She was thanked for all her work. Volunteers for Chair were requested.

9. Dates of next meeting

9 June 2023

There was a strong preference for in-person meetings.

Actions from this meeting

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ISIS to progress User Charter	Ongoing	Philip / Emma G	Jan 2022
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ISIS Neutron and Muon Source

Development of IUC involvement in NMSUM	New action	Philip, Ross, David	Dec 2022
Experimental reports – revised question set and submission rate	New action	Philip	Dec 2022
ORCID capture and use	New action	Emma	Dec 2022
Students as PIs on proposals – check Diamond’s experience and action	New action	Emma	Dec 2022
DOI for multiple datasets / raw and reduced data	New action	Hannah	Dec 2022
IDaaS information on the ISIS website and provision of computing information in general	New action	Hannah	Dec 2022
Videos on data analysis	New action	Philip / Hannah	Dec 2022
Video on Data Gateway	New action	Hannah	Dec 2022
RAL site map on ISIS website	New action	Emma	Dec 2022
web information on sample environment equipment and access	New action	Marek	Dec 2022
report back on access to biolab and equipment.	New action	Marek	Dec 2022
Inter step and lighting	New action	Marek	Dec 2022
List of user meeting dates to be created	New action	Philip	Dec 2022