

ISIS Neutron & Muon Source User Committee

6 Dec 2019, The Cosener's House Abingdon, 10-00 – 13-00.

Present:

- IUG1 Crystallography
 - Karen Johnston (Durham)
 - Michael Hayward (Oxford)
- IUG2 Disordered Materials
 - Emma Barney (Nottingham)
- IUG4 Excitations
 - Chris Stock (Edinburgh)
- IUG5 Molecular Spectroscopy
 - Roberto Senesi (Rome)
 - Alexander O'Malley (Bath)
- IUG 6 Muons
 - Lucy Clark (Liverpool)
 - Joseph Wright (UEA)
- IUG7 Engineering
 - Catrin Davies (Imperial)

Sean Langridge – ISIS Diffraction & Materials Division Head

Philip King – ISIS Spectroscopy & Support Division Head

Zoe Bowden – Head of ISIS Operations

Steve Wakefield – representing ISIS Experiment Operations Division

Andrew Kaye – User Programme Manager

Hannah Griffin – Computing Division Head

Matt North – Experimental Operations Division Head

Apologies:

- IUG2: Disordered Materials
 - Paul Bingham
- IUG3 Large Scale Structures
 - Tim Knowles (Birmingham)
 - Aiden Hindmarch (Durham)
- IUG4 Excitations
 - Kelly Morrison
- IUG7 Engineering
 - Richard Moat

The meeting opened with introductions by all present.

1. Minutes from the June 2019 IUC meeting

These were approved with no comments.

2. Actions arising from previous meetings

Action from previous meeting and status	Status	Responsible	Meeting action added
Consider review of archaeometry proposal assessment.	<i>FAP has suggested setting aside time for Archaeometry proposals so that they are in competition with each other not with the engineering proposals. Further discussion with the archaeometry community necessary.</i> Ongoing.	Philip King	Dec 2018
Update the IUC at the next meeting on staff being able to load cash onto their cards.	<i>This is practical to do, but has an associated cost. Andrew Kaye to continue to progress.</i> Ongoing.	Andrew Kaye	Dec 2018
Raise the hotness of food and long till queues.	<i>Monthly meeting with catering manager and user office. Issues are being raised.</i> Done.	Andrew Kaye	Dec 2018
Add DOI reference format to web page	<i>DOI postcard produced, website updated.</i> Done.	Philip King	June 2019
Explore with HZB whether any of their high field magnets (not at the highest extremes of field) might be available	<i>There has been active exploration of this with HZB. It's not clear ISIS can benefit from HZB magnets, but we may get a dilution fridge from HZB in the new year.</i> Done.	Philip King to ask Steve Wakefield	June 2019
Send round to ISIS scientists the sheet describing what's appropriate for Xpress measurements and put this online	<i>Xpress description available on the ISIS website</i> https://www.isis.stfc.ac.uk/Pages/Xpress-Measurements.aspx Done.	Philip King	June 2019
Explore whether creating bank statements at departmental level is possible.	<i>Website modified to say we'll respond to individual requests from users or departments for this information, which can be easily produced if required</i> Done.	Philip King	June 2019
Ensure summary bank statements are sent to users for the full REF period	<i>Statements sent this week.</i> Done.	Philip King	June 2019
Consider Ken Anderson at next year's NMSUM meeting	<i>Ken no longer at the ESS.</i> Done.	Philip King	June 2019
Enable reps for SANS and reflectometry for next IUC meeting	<i>AK to give names of new SANS and reflectometry IUC reps.</i> Ongoing.	Philip King	June 2019
Consider online template, examples of good proposals and additional information in the proposal system to encourage improvement in proposal writing	<i>Template is available as Word doc and as a web page.</i> <i>Example proposals to be done.</i> Ongoing.	Philip King	June 2019
Explore whether the OSNS session on proposal writing could be videoed.	<i>Videoing the OSNS session is probably not possible. But session on proposal-writing to students being considered for student day / NMSUM.</i> Ongoing.	Sean Langridge / Philip King	June 2019
Philip King to invite Lamar and/or new Scientific Programme Manager to next IUC to update on software strategy.	<i>We will do this for the next IUC meeting. Toby Perring has just started as Scientific Programme Manager – he'll be able to give a better update in the summer.</i> Ongoing.	Philip King	June 2019

3. Reports from user groups

UG1 - Crystallography:

A recent very successful user group meeting took place at Milton Hill – 110 participants over 2 days. Thanks to Helen Playford and others for the organisation. There looks to be a good publication list on Epubs from crystallography instruments so far this year so far. Survey results show a high level of user satisfaction with the crystallography programme, with some suggestions for on-site facilities: Deuteration facility – can users have an analysis of sample before measurement, for example? The new HRPD setup looks very good and much more inhabitable; the community continue to support the full instrument upgrade. There is an ongoing request for software support for total scattering.

Action: Steve Wakefield to consider characterisation of deuterated samples produced by D-Lab.

UG2 – Disordered Materials:

Paul had solicited comments from community, although hadn't received many responses.

Comments from John Holbrey and Paul:

- 1) Silvia Imberti left in June to take up a job outside of STFC. Hopefully she will be / has been replaced. [to note that Oliver Alderman has started at ISIS as Silivia's replacement].
- 2) Preparations for the SANDALS upgrades in parallel with the big TS1 shutdown should be progressing.
- 3) There is a Disordered Materials User Group meeting from Tuesday 21st to Friday 24th January 2020 at Cosener's House, Abingdon. The meeting is now fully booked which is excellent news and it promises to be a very good event.
- 4) Tristan Youngs will be unveiling his 'Dissolve', a new development to advance on the capabilities of EPSR for modelling structure which uses more chemically understandable parameterisation (using a genuine force field with bond/angle/dihedral descriptors).

UG3 – Large Scale Structures:

No report.

UG4 - Excitations:

There have been positive comments on new upgrade to Mari, and good comments on sample environment provision. There is an issue around being able to view data during experiments on the beamline: IDaaaS is liked when it works, but there are issues around login and operations. [Whilst new nodes to support IDaaaS operations have been bought recently, ISIS is aware of operational issues, and the operational support model is continuing to be developed]. There was a question over ISIS Compute not working fully. The community are keen to see the Wish magnet back [it is now back at ISIS and needs a little more further work, but should be operational from the new year]. Issues with DAE-3 were raised – ISIS was not aware of generic issues, though a particular problem on Mari had been solved.

Action: Hannah Griffin to look at ISIS Compute issues.

UG5 – Molecular Spectroscopy:

The next User group meeting will be 8-9 sept 2020 at Coseners, and will focus on industrial use and simulation. The Good Vibrations newsletter goes out twice per year with 600+ recipients. There will be a special issue of J. Comp. Phys. on computing in neutron scattering with an emphasis on quantum, molecular and classical modelling applied to neutron scattering; this will be online soon with Jeff Armstrong and other as editors. Experimental support comments are positive. A controlled humidity chamber has been requested by several groups. More tailored sample cans for Vesuvio and Tosca for top-loading have been requested. Automated gas manifold has been a long-time request; purchase of commercial system is now being considered and this seems a good way forward, likely to satisfy most requirements. Two new PhD students have been appointed in conjunction with the catalysis hub, with Loughborough and Glasgow, and will start in the next academic year; a call for one further student project will be made soon.

Action: Steve Wakefield to check on sample can requests.

UG6 - Muons:

SuperMusr feasibility is continuing. MuX for elemental analysis is also undergoing detector exploration. New solenoid for RIKEN is also being flagged.

UG7 - Engineering:

A User meeting took place over 2 days in December. For the furnace, temperature measurement needs a look at, as calibration may be an issue. There were some detailed comments on other aspects of sample environment and storage – a request for environmental control for storage of architectural items. Very positive comments on instrument scientists, and appreciation of flexibility for recovering beamtime when ISIS goes down.

Action: Catrin to talk with instrument scientists about calibration data.

Action: Catrin to ask instrument scientists whether this is a more general request.

4. Update from ISIS

Zoe Bowden gave an update on ISIS, including:

- New Computing and Experimental Operations division heads
- New Instrumentation Development Group
- Appointment of Toby Perring as new Scientific Computing lead and Programme Manager
- Deuteration facility – 500th deuterated material produced
- Delivery of new muon sub-1K equipment
- SINE2020 EU project SE developments and network
- 10,000th ERA approved this cycle
- Image database available
- Proton pulse compression for muons
- Detector developments
- Instrument control – rollout of IBEX system
- User programme and scientific software
- Endeavour instrument programme
- Large number of schools and meetings over the past year
- Public engagement events
- Proposal numbers increasing
- Long shutdown planning

5. Communications with the user community

Following an introduction on the paper circulated in advance, there was general discussion regarding ISIS communications with the user community. Ideas included:

- Making workshop material available to those not present.
- Video tutorials on software (good x-ray examples)
- e-learning: making sure we're publicising well the material that we have got (web links, etc), in addition to generating new materials.
- Using Twitter much more: for publicising resources; tweeting ISIS deadlines ('5 sleeps till the next proposal deadline') and countdown tweets; tweeting the proposal template and example proposals; using twitter for polling users, getting conversations going on particular topics . . .
- Distribute ISIS poster to users for putting up in departments
- Material for users to talk about ISIS . . . develop this further, publicise it more, add link to image database (or put additional images up if this isn't available externally)
 - Action:** Philip to check on image database external visibility
- Is Slack externally available for users?
 - Action:** Hannah Griffin to check
- Use STFC linkedin account

- Use Tiktok

6. ISIS Data Policy

Following an introduction on the paper circulated in advance, there was general discussion regarding issues around the ISIS data policy. Ideas included:

- Most users can't access LET/MARI etc data files as they're so big. Users rely on ISIS systems at all steps. It is very difficult for users to take Tb of data away and store on university systems.
- It was noted that reduced IN5 data from ILL can't be stored on ILL systems and so ISIS systems may be being used for this.
- An ideal lifetime of big files (reduced data) was thought to be 3 years – equivalent to a PhD length.
- Can Python script files be kept forever?
- Could larger files be stored on tape? – OK if they take a bit longer to come back.
- The 3 year embargo period for ISIS data was felt to be appropriate.
- Collection of metadata was discussed. It was noted that some xpdf instruments ask for metadata in advance of runs. ISIS could at least make sure we have a system whereby full metadata can be captured if users want to do this. Is metadata fully available through ICAT?

Action: Hannah to check on current metadata system and how metadata is available.

7. Update on Machine Operations

- Steve Wakefield provided details of ISIS operating over the past 6 months, including a look at major issues such as linac tank 4 RF window failures and an ion source failure.
- Works in the halls including lighting replacement were discussed
- The Experiment Risk Assessment system was discussed – this was a major cultural change introduced 10 years ago, and the IUC (of that time!) was thanked for supporting the measure. It has just reached the 10,000th ERA.

8. Update on ESS

Sean Langridge gave a description of the current status of the UK contribution to the ESS, focusing on UK instrument progress: Loki (broadband SANS instrument) and Freia (reflectometer).

9. AoB

- The introduction of User Coffee and Cake was noted
- The new requirement for users to say which organisation was responsible for them whilst they are at ISIS was also noted, with a new tick-box page being introduced into the safety test online system.

10. Date of next meeting

It was agreed that the next IUC meeting would be Mon 8 June, joint with FAP Chairs, in Warwick at NMSUM. [Note added subsequently: this arrangement may change due to the implications of the delay to the ISIS long shutdown – IUC members will be contacted with revised plans].

11. Summary of actions arising and ongoing:

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Consider characterisation of deuterated samples produced by D-Lab.	New action	Steve Wakefield	Dec 2019
Look at ISIS Compute issues	New action	Hannah Griffin	Dec 2019
Check on sample can requests for Tosca, Vesuvio	New action	Steve Wakefield	Dec 2019
Discussion with instrument scientists on engineering furnace calibration data and whether storage with environmental control is a more general need.	New action	Catrin Davies	Dec 2019
Check on image database external visibility	New action	Philip King	Dec 2019
Check on availability of SLAC MCR news for users	New action	Hannah Griffin	Dec 2019
Check on current system for collecting metadata for ISIS experiments and how metadata can be accessed subsequently	New action	Hannah Griffin	Dec 2019