

## ISIS Neutron & Muon Source User Committee

7 June 2019, The Cosener's House Abingdon, 10-00 – 13-00.

### **Present:**

- IUG1 Crystallography
  - Emma McCabe (Kent)
  - Michael Hayward (Oxford)
- IUG3 Large Scale Structures
  - Aiden Hindmarch (Durham)
- IUG4 Excitations
  - Chris Stock (Edinburgh)
  - Kelly Morrison (Loughborough)
- IUG5 Molecular Spectroscopy
  - Roberto Senesi (Rome) – **Chair**
  - Alexander O'Malley (Bath)
- IUG7 Engineering
  - Catrin Davies (Imperial)
  - Richard Moat (Open University)

Sean Langridge – ISIS Diffraction & Materials Division Head

Philip King – ISIS Spectroscopy & Support Division Head

Zoe Bowden – Head of ISIS Operations

Marek Jura – representing ISIS Experiment Operations Division

### **Apologies:**

- IUG2: Disordered Materials
  - Paul Bingham
  - Emma Barney
- IUG3 Large Scale Structures
  - Tim Knowles (Birmingham)
- IUG6 Muons
  - Nicola Morley (Sheffield)
  - Martin Lees (Warwick)

The meeting opened with introductions by all present.

### **1. Minutes from the Dec 2018 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 short Xpress reports and how these can be captured	<i>Will be done once experiment report system is made online</i>	Andrew Kaye	June 2017
Set up a mechanism with Philip for looking at user comments on software, and specifically explore the issue of processing of PDF within Mantid (and whether SNS have implemented anything).	<i>To be done</i>	Debbie Greenfield	Dec 2018
Explore GSAS software on Engin-x and whether latest versions are being used.	<i>Done: Conversations ongoing with Bob von Dreele. Hope to link with Diamond in this area. Some scripting has gone into Mantid.</i>	Sean Langridge	Dec 2018
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>	Philip King	Dec 2018
Explore NERC support for archaeometry proposals.	<i>Done: Philip has been in touch with Nicola Lewis, the programme manager at NERC with responsibility for the archaeometry area, and passed her details to Adrian Hillier to follow up on.</i>	Philip King	Dec 2018
Update the IUC at the next meeting on staff being able to load cash onto their cards.	<i>Ongoing discussions with estates.</i>	Andrew Kaye	Dec 2018
Check that the bar facilities are still operating during evenings at Ridgeway.	<i>Done: bar open 7pm to 11pm</i>	Andrew Kaye	Dec 2018
Raise the hotness of food and long till queues.	<i>Done. Self checkout for barcode items suggested; queuing in the evenings may still be an issue.</i>	Andrew Kaye	Dec 2018
Put NMSUM update talks online after the meeting.	<i>Done. Talks are linked from the 2019 NMSUM meeting page, and a news item on the ISIS website gives people the dates of the 2020 meeting (8-10 June 2020).</i>	Philip King	Dec 2018

### 3. Reports from user groups

#### **UG1 - Crystallography:**

Given the regular oversubscription of the Crystallography User Group meeting (held jointly with BCA's PCG and IOP's SCMP winter meeting), this meeting will take place in the larger venue of Milton Hill House, as in 2018, which worked well. The meeting will be held on November 4th-5th. As in 2018, we'll include input from the "Physical Sciences" group from Diamond Light Source; discussions are currently taking place to ensure stronger engagement from Diamond than last year (liaising both with "Physical Sciences" and "Crystallography"). An international meeting on "High pressure neutron diffraction: current and future prospects" was also held in Abingdon in May and brought together UK, EU and US researchers.

There have been ~66 publications (listed on the STFC epubs database) associated with ISIS Crystallography instruments (GEM 1; HRPD 1; PEARL 15; POLARIS 5; SXD 7; WISH 22) published so far in 2019 (61 at this point in 2018).

The community has a high level of user satisfaction with the instruments and with expert help from instrument scientists. We're glad that the interim restoration project on HRPD has begun and the user community looks forward to using the "restored" HRPD in September. Again there was a comment on ease of use of software for total scattering, but there are plans within the group to develop this further. There were some difficulties reported with sample environments (e.g. temperature control above room temperature, and a dilution fridge experiment).

This panel round has seen 194 proposals – significantly more than usual. WISH is heavily oversubscribed, which illustrates how competitive it is to be allocated time on this. With this in mind, it's a shame that with the 14 T magnet not yet fixed, there are a number of highly rated proposed experiments from previous rounds that can't be scheduled on WISH. We continue to see many experiments requiring complex sample environments (in situ/in operando measurements) across a range of instruments across a number of instruments. Some experiments have been allocated time in previous proposal rounds but have not been scheduled due to lack of technical support for gas handling/high pressure; it would be a shame for ISIS to lose this science if users take these experiments elsewhere.

The group really values NMSUM which brings so much of the community together. One idea from the panel is to include a session on proposal writing aimed at early-career researchers (e.g. perhaps on the student day). If whoever led this session was happy to be recorded (as is the norm for most university teaching now) and the video put online, this could be a useful resource for new users, both within the UK and globally. (*see further discussion of this below*).

#### **UG2 – Disordered Materials:**

1) In an effort to reach out to as wide a range as possible of the Disordered Materials community to gain their feedback, Paul Bingham contacted all beamline scientists relevant to FAP-2, and also contacted the User Office to access users, inviting input and feedback. This led to email sent out on 30<sup>th</sup> May by the User Office inviting feedback from across the community and signposting the relevant. Many thanks to the User Office for this – it should become a permanent feature of IUC meetings.

Feedback from Daniel Bowron:

2) This is the last proposal round in which SANDALS will be taking submissions until after the long shutdown. The work on the SANDALS incident flight line collimation, front end shielding and frame overlap chopper is planned to start in January 2020, so we are only operating until the end of the December 2019 cycle. SANDALS will thus be offline from January 2020 until November 2021, but should come back with improved incident beam collimation, new beam defining apertures and a frame overlap chopper to improve signal to background.

- 3) NIMROD is operating well. We hope to bring its long awaited improved gas handling panel into service in the forthcoming cycle (June 2019). We are also working on putting together the sample imaging neutron camera that we have designed to be installed inside the vacuum tank. When this is installed, we will be able to drive the camera up from the base of the sample tank to directly image the sample. This should help us monitor things such as filling fluids into porous materials, as well as check on beam positioning on complex sample configurations.
- 4) GEM is working reasonably well. There are currently a few issues with increased numbers of failing detectors on its array, but this is currently being investigated as we don't want to suddenly find that we lose whole banks due to the complex encoding that links the many detector elements on the instrument.
- 5) Our two laboratory XRDs are seeing good service. The newer Malvern-PANalytical Empyrean system has recently had its pixellated detector refurbished as this failed following a software update. Thankfully things seem to be operating well once again since it was fixed a couple of months ago. The older PANalytical Xpert Pro system currently needs to have its Ag-tube replaced to restore operating flux, but that is something that we hope to get onto when we have a bit of free time.
- 6) On the software front, Tristan has been working hard on developing "Dissolve" as a next generation version of Alan's Empirical Potential Structure Refinement code. He is currently writing up the project documentation to support the 120k lines of code he has already written, with the aim of making this a formal project within the ISIS portfolio of software activity. In the meantime, the group is still basing the majority of our modelling activity around standard EPSR. From what we have seen of the new code, it is certainly looking very promising - it can already replicate what EPSR can do for standard neutron studies of liquids and glasses, but it is capable of million atom plus modelling, whereas standard EPSR tops out at around about 150k atoms. This all bodes well for providing the modelling tools to take full advantage of the 30nm length scale capability of NIMROD which requires models in the 3 million to 5 million atom range.
- 7) The community is making increasing use of the ISIS deuteration facilities, although we do need to take care to communicate and coordinate our instrument scheduling with the delivery of essential components that they synthesise for us. Limited staffing in the D-lab, largely due to maternity leave, has left them a little short staffed at times in the past six months, but hopefully they will be back up to full operational capability very soon.

Feedback from John Holbrey:

- 8) The Neutron/Muon meeting in Warwick at Easter was good, the range of science discussed was appreciated. John's group has conducted several experiments over the past year, with excellent support from beam scientists, D-lab, and user office for logistics (credit all round).

### ***UG3 – Large Scale Structures:***

- A user meeting was held at end of Nov 2018 which was well attended with excellent talks; the plan is for this to happen every 2 years.
- In the user feedback there are lots of good comments on instruments and instrument scientists. No complaints about the coffee machines (!).
- The splitting of the LSS FAP panel into SANS and reflectometry panels seems to have worked well – this seems the right way of splitting the FAP compared with splitting along science lines (soft matter and magnetism).
- The NMSUM meeting was good, and there the split by science rather than technique seems to work well.
- Current upgrades on TS2 LSS instruments look good and are welcomed, along with investment in characterisation labs.

#### **UG4 - Excitations:**

- The Mari upgrade is now complete giving an order of magnitude increase in low energy neutron flux.
- A polarisation option on LET is now in user programme.
- The workshop on Horace & Spin-W in Jan 2019 were appreciated as simulation and analysis of data is often a bottleneck.
- In the user feedback it was nice to see only a single issue with the dilution fridge, though stability of the system looks still to be an issue. One user had raised the possibility of instrument schedules being available online – there was discussion of this, and some concern that visits information shouldn't be publicly available. One user had suggested that it would be good to have more data reduction script examples available on line.
- The Maps upgrade is working well.
- The closing of HZB was discussed in terms of whether there are opportunities for ISIS to expand its high-field programme, possibly by us seeing if some of the HZB magnets might be available (in the sub-20T region).
- There were comments from a few users to say that they had got 80% of the data they needed in some cases, but getting time from the panels for the additional data needed was a problem. ISIS noted that panels are always encouraged to give enough time for experiments to be completed.
- The PACE & Symphony projects are seen as good; but on-beam viewing & analysis of data is a problem. Some issues with iDAaaS reliability.

**Action: Steve Wakefield to explore with HZB whether any of their high field magnets (not at the highest extremes of field) might be available**

**Action: Philip King to send round the sheet describing what's appropriate for Xpress measurements and put this online.**

**Action: Philip King to invite Lamar and/or new Scientific Programme Manager to next IUC to update on software strategy.**

#### **UG5 – Molecular Spectroscopy:**

- Planning for the next Molecular Spectroscopy User Group meeting is underway – this will be at the Cosener's House next summer. The UG Meeting held at UCL was good, and there is an idea to alternate between Cosener's and a university location, with Bath being suggested as host for the one after next.
- There was good feedback overall from user comments.
- A controlled humidity chamber, either offline or as a stick attachment – had been suggested and might benefit a number of users. It was hoped that the pressure rating for cells on Tosca could be increased. There is a request for an automated gas-handling system. No current issues with Mantid were raised, and the problem of adding runs together had been fixed.
- The number of new PIs was good.
- The next MDANSE meeting in 2020 would be held at the ESS.
- There is a QENS and reflectometry workshop at Imperial next week.
- Good Vibrations, the user group newsletter, goes out to 650 recipients before each proposal round.
- There is a plan to produce a user-centric document illustrating the Tosca upgrade with clear before/after illustrations for users to show the new science now possible.

#### **UG6 - Muons:** (report received after the meeting):

##### Points to note

- Dilution fridge is still required on HiFi
- Higher time resolution (MuSR – pulse slicer, and on HiFi)
- LABS: a microscope would be useful new the muons, and the helium glovebox should be maintained

- Ridgeway house: issues with mould in the bathrooms.

#### Comments about the Muon facilities:

- RIKEN-RAL in the new agreement until 31<sup>st</sup> March 2023, with significant refurbishment during the long shut down
- Want to grow the MuX – elemental analysis technique, as it has a growing user base, to do this a new design would be implemented that would improve the flux by x100
- Dilution fridges: have ordered 4x dilution inserts, 2x He3 inserts and 2x new cryostats, but have only received one cryostat, stick and He3 insert, rest are due, but the base temp is higher than the spec
  - o This has caused issues with the user program and have over 30 days of carryover

#### Upcoming meetings:

- Muon advanced school 2019, 28 Aug – 6 Sept 2019 at RAL
- 15<sup>th</sup> International Muon conference, 6-10<sup>th</sup> July 2020 at Univ. of Parma, ISIS group is jointly organising it

#### UG7 - Engineering:

- User comments had given praise for instrument scientists; there were some complaints about beam downtime, but examples of this had been dealt with well by ISIS staff with extra time and support given.
- There is continued concern regarding Engin-x software which is dated.
- The recent panel meeting had seen lots more engineering proposals, but some poor quality.

## 4. Update from ISIS

Points from Zoe Bowden's talk included:

- The recent increases in proposal numbers (particularly from India, China and Sweden); and the increase in use of Rapid and Xpress routes
- The increase in publication numbers for 2018 (it was suggested that this may be due to the upcoming REF as well as instrument number increases)
- Brief descriptions of current instrument upgrades, including Mari guide and detector electronics; Zoom now in the user programme; the variety of science on Imat; the successful start of industrial usage of Chiplr; the HRPD intermediate upgrade; the GEM jaws and alignment upgrade; the availability of polarisation on LET; Sandals chopper work; the RIKEN-RAL refurbishment.
- A brief update on funding bids for the Endeavour instrument project
- Plans for feasibility studies for ISIS-II
- Plans for the long shutdown, including TS-1 refurbishment and Linac Tank IV replacement.
- Overseas partnerships update
- Engagement with students

In discussion, it was commented that, when the HRPD upgrade had to be pushed back recently, thanks should be given to the beamline scientists for enabling the time created to be used well.

DOIs were discussed – the correct referencing format needs to be added to the ISIS DOI page.

**Action: Philip – add DOI reference format to web page**

It was commented that improvements to the WIFI service on site had been noticed and appreciated, including the Eduroam connection being improved and more reliable.

REF processes were discussed. The user 'bank statements' are appreciated. Having these available at departmental level may be beneficial.

**Action: Philip to explore whether creating bank statements at departmental level is possible.**

**Action: Philip to ensure summary bank statements are sent to users for the full REF period.**

## 5. Update on ISIS Machine Operations

Marek Jura gave the update. Delivery in 18/19 year was described. There had been some dip in availability and a summary of major beam outages was given.

## 6. Overview of support lab facilities at ISIS

Marek described the ISIS support labs:

- Deuteration lab – the no. proposals, the lab capabilities and the nature of materials produce, the instruments within the ISIS suite covered by deuteration requests was noted (5 different FAPs) plus material for ILL proposals. Science highlights from the deuteration programme were shown, and interactions with users including the recent deuteration user meeting, and hosting students and post-docs.
- Materials characterisation lab – this is very well used; there had been a recent obsolescence programme to replace obsolete kit; a new PPMS system (end 2019) including dilution fridge had been purchased and the single crystal diffractometer replaced. 18 months ago a new magnetic property measurement system with <sup>3</sup>He insert was provided.
- Chemistry and catalysis lab – glove boxes have been an issue, and existing ones have been refurbished as well as a new glove box purchased just for sample storage – this is installed in R80 next to Wish, and the possibility of getting a second for TS1 is being explored.
- R79 Hydrogen & catalysis lab has been refurbished, and the high throughput robot has been decommissioned to make space for preparation work

In discussion, the possibility of extending use of the crystal growth lab was considered, and there was considered to be a need for this to complement other capability in this area in the UK. Discussions are ongoing with Diamond as to whether they would also like to support a modest extension of the lab's capabilities.

## 7. Feedback on the NMSUM Meeting

- It was felt to be a good meeting, appreciated by users. The science day categories were good and about the right number.
- ESS engagement with UK community was discussed, and getting the balance right on this in terms of managing expectations at the present time whilst fostering interest.
- Ken Anderson could be asked to talk at NMSUM about the ESS instruments more directly  
**Action: Philip to consider Ken Anderson at next year's NMSUM meeting**
- There was generally good feedback from student day.

## 8. AoB

Now that the LSS group and FAP had been split into reflectometry and SANS, it was suggested that the IUC have two reps for each of these areas.

**Action: Philip to enable reps for SANS and reflectometry for next IUC meeting.**

Early career researcher experience at FAPs: There was discussion on giving early career researchers experience on proposal writing by allowing them to sit on FAPs. This could be done by having one student present per FAP and that person reporting back on what they had learnt at student meetings; but there was also concern about confidentiality at the FAPs. Other suggestions for enabling students (and others) to develop proposal-writing skills included improving the online 'template' for the science case; putting

examples of good proposals online; providing a lecture/tutorial on proposal writing at a student meeting, videoing this and making the video available online; or the session at the Oxford School on proposal writing could be videoed. Additional information could also be added into the proposal system. It was noted that different panels have slightly different expectations of what is required in a proposal.

**Action: Philip to consider online template, examples of good proposals and additional information in the proposal system**

**Action: Sean to explore whether the OSNS session on proposal writing could be videoed**

## 9. Date of next meeting

The next IUC meeting is Fri 6 Dec 2019.

## 10. Summary of actions arising and ongoing:

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>	Philip King	Dec 2018
Update the IUC at the next meeting on staff being able to load cash onto their cards.	<i>Ongoing discussions with estates.</i>	Andrew Kaye	Dec 2018
Raise the hotness of food and long till queues.	<i>Done. Self checkout for barcode items suggested – this to be explored</i>	Andrew Kaye	Dec 2018
Add DOI reference format to web page		Philip King	June 2019
Explore with HZB whether any of their high field magnets (not at the highest extremes of field) might be available		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		Philip King	June 2019
Explore whether creating bank statements at departmental level is possible.		Philip King	June 2019
Ensure summary bank statements are sent to users for the full REF period		Philip King	June 2019
Consider Ken Anderson at next year's NMSUM meeting		Philip King	June 2019

Enable reps for SANS and reflectometry for next IUC meeting		Philip King	June 2019
Consider online template, examples of good proposals and additional information in the proposal system to encourage improvement in proposal writing		Philip King	June 2019
Explore whether the OSNS session on proposal writing could be videoed.		Sean Langridge	June 2019
Philip King to invite Lamar and/or new Scientific Programme Manager to next IUC to update on software strategy.		Philip King	June 2019