

## MINUTES OF MEETING

**Title/Subject:** Diamond User Committee Meeting #11

**Venue:** Diamond House, G53/4

**Chairman:**

Dr David Lawson

**Time/Date:** Tuesday 23<sup>rd</sup> September 2014

**Secretary:**

Kathryn Poulter

### PARTICIPANTS

### ADDITIONAL DISTRIBUTION

#### DUC members

Alan Dunbar  
David Lawson (Chair)  
Peter Lee  
Rob Lindsay  
John McGeehan  
Feodor Ogrin  
Peter Wells  
David Dye  
Josep Sule Suso  
Joe Hriljac

#### Institution

University of Sheffield  
John Innes Centre  
University of Manchester  
University of Manchester  
University of Portsmouth  
University of Exeter  
Research Complex at Harwell  
Imperial College of London  
Keele University  
University of Birmingham

#### Diamond Light Source representatives:

Alun Ashton  
Sarah Bucknall  
Gianfelice Cinque  
Andy Dent  
Michael Drakopoulos  
Rob Walton  
Dave Hall  
Mark Heron  
Susan Judge  
Burkhard Kaulich  
Chris Nicklin  
Kathryn Poulter  
Bill Pulford  
Trevor Rayment  
Kawal Sawhney  
Cecilia Sanchez-Hanke  
Dave Stuart  
Richard Walker  
Martin Walsh  
Silvana Westbury  
Jorg Zegenhagen

Data Analysis Software Group Leader  
Scientific Communications Co-ordinator  
Soft Condensed Matter Village Coordinator  
Physical Sciences Coordinator  
Engineering & Environmental Science Village Coordinator  
Data Acquisition Group Leader  
MX Village Coordinator  
Controls Group Leader  
User Office Manager  
Spectroscopy Village Coordinator  
Surfaces & Interfaces Village Coordinator  
Operations Programme Manager  
Scientific IT Software Computing Coordinator  
Director, Physical Sciences  
Materials Village Coordinator  
Scientific Operations Coordinator  
Director, Life Sciences  
Technical Director  
Life Sciences Coordinator  
Interim Head of Communications  
Physical Sciences Coordinator

**Apologies:**

Liane Benning

Tom Hase

University of Leeds

University of Warwick

## 1. INTRODUCTIONS AND OPENING REMARKS

Dave Lawson welcomed everyone to the meeting

Apologies were received from Liane Benning and Tom Hase.

## 2. MINUTES AND ACTIONS

The Minutes of the meeting held on 18<sup>th</sup> March 2014 were approved.

Action 8.2 – Diamond will consider how best to move forward regarding sending outlook appointments with beamtime allocations. An update will be provided at the next DUC.

**Action: Bill Pulford**

Action 8.13 – The best documentation to use regarding data backup is on the MX webpages. This will be made more widely available on the web.

**Action: Bill Pulford**

Diamond is still looking to improve external network connections and is working with STFC on this. An update will be provided at the next DUC.

**Action: Bill Pulford**

Action 8.14 – Clarification of the process for multi disciplinary applications is moving forward. Cecilia commented on behalf of Martin Walsh, that in the current UAS it is not possible to make a multi-disciplinary application yet, except MX bags can apply for SAXS time through UAS.

Action 10.3 – Sue confirmed that there is now more information on the Peer Review Process on the web. Sue will send out the link, and any feedback would be appreciated.

**Action: Sue Judge**

All other actions were completed.

## 3. HEALTH & SAFETY

There were no issues raised.

## 4. ESUO

David Lawson provided an update on this organisation. Their main remit is to secure EU funding to support transnational access (TNA). The funding for renewal is being looked at but under Horizon 2020, purely TNA is not permitted, and so a new strategy is required. Lobbying materials are being prepared to help national EU delegates support the case for TNA.

There will be a meeting next week in Lund to discuss how to structure the next proposal. Peter Fletcher from STFC is the lead UK delegate on the Research Infrastructures Programme Committee. The future of the ESUO is in the balance until further funding can be secured.

Trevor reported that a brochure has been published to promote the success of transnational access which he will circulate.

**Action: Trevor Rayment.**

## 5. ENGAGEMENT WITH USER COMMUNITY

David Lawson commented that the level of feedback received from the community is low, and questioned whether there was a better way of achieving this.

Methods to take this forward need to be useful and not too onerous. Several options were considered: -

- Carry on as we are
- Target particular issues
- Online survey
- Face to face interviews with selected users
- A satisfaction survey incorporated into the UAS
- Give delegates at the User meeting a hardcopy questionnaire to complete
- Provide incentives for completing surveys

The overall view of the committee was that users were generally happy and this was reflected in the low level of feedback. It was agreed that prior to DUC meetings, the representatives would continue to seek user feedback through emails targeted to their respective villages.

End of experiment forms pick up a lot of feedback from users. These are reviewed at an internal meeting, and anything graded poor is responded too. Trevor and Dave agreed to review the process regarding how Diamond responds to end of expt form feedback, and agree in consultation with Dave Lawson how this can best be used by the DUC.

**Action: Trevor Rayment & Dave Stuart.**

## 6. MACHINE UPDATE REPORT

Richard Walker gave a presentation to update the DUC on developments and performance of the machine. Following the recent RF cavity change, the expectation was that the machine would be run at ~200mA, and the current built up from there as soon as possible depending on reliability.

## 7. PHYSICAL SCIENCES REPORT

Trevor Rayment gave a presentation to update progress on the Physical Sciences beamlines.

## 8. LIFE SCIENCES UPDATE

Dave Stuart gave a presentation to update progress on the Life Sciences beamlines.

The mail-in service for BIOSAXS was discussed. Dave suggested that users get in touch with Rob Rambo (Principal Beamline Scientist on B21) directly to discuss opportunities, and also if they are keen to receive training.

## **9. USER OFFICE REPORT**

Sue Judge gave a presentation to update the DUC on the user office and the new UAS system.

## **10. SOFTWARE REPORT**

Rob Walton gave an update on the Data Acquisition group's activities over the last year. The implications for backing up data if it is in NeXus format were discussed especially if file sizes were larger than some (portable) backup media and the files would need to be split over more than one device. Rob replied that discussions with detector manufacturers including Dectris were ongoing with many problems arising from the change being discussed. The drive towards NeXus is particularly for physical science beamlines in the first instance though the nature of some newer detectors could make this a necessity from a data throughput perspective on any beamline.

The advantage of using NeXus, which uses a standard for additional information of the experiment, is that we can use it as a basis to go forward and develop analysis software that is as automated as possible. An additional advantage is that in the nexus file you can have a complete record of what has been done to the data to get to a diffraction pattern, i.e. calibration, process etc.

As detectors get faster, writing a file for each exposure becomes less practical as creating files is an expensive thing for a filesystem. Moving toward writing NeXus files allows detectors to write multiple images into an hdf file which can then be linked from a NeXus file. There are currently no plans to change MX to writing NeXus but future detector technology may make it a requirement.

## **11. COMMUNICATIONS UPDATE**

Sarah Bucknall gave an update on this year's SR user meeting. Feedback and suggestions for next year would be welcome. Comments should be sent to [events@diamond.ac.uk](mailto:events@diamond.ac.uk)

Silvana Westbury gave an update on the PhD Investigator award and an outline of the opportunities there are for Users to work with the comms team.

## 12. FEEDBACK FROM VILLAGE COORDINATOR BREAKOUT SESSIONS

### 12.1 MX

There were a number of comments that were discussed in detail in the session relating to software, and the responses will be communicated to the individuals.

The tracking of hard drives sent with dewars is not as robust as it could be. Sometimes they have gone astray (although they have eventually been tracked down). This represents a potential data security risk. Diamond will review procedures for hard drive tracking and report at the next meeting.  
**Action: Dave Hall**

It was suggested that if the FTP option could be more robust then hard drives wouldn't be needed. Mark Heron reported that there is a plan to install a temporary server outside the firewall which should make a significant difference. A final network solution is approx. 12 months away.

The position of the rotation axis is checked daily, however sometimes users adjust this rather than speak to the local contact if they suspect a problem. Diamond to review whether this function should be greyed out or password protected.  
**Action: Dave Hall**

There is a concern about unsupervised inexperienced remote users. One solution would be that each remote site must have at least one experienced user present during data collection. However this is difficult to police. Other suggestions were for Diamond to consider running more BAG training (as this is oversubscribed), to review the guidelines for remote users and to consider producing an online video of the "ideal data collection session" for training purposes.  
**Action: Dave Hall.**

### 12.2 Soft Condensed Matter

It was asked whether the checkout time from Ridgeway could be 12pm as the default? It is possible for users to ask for a later check out but this cannot be guaranteed. It was agreed that the User Office would discuss this matter further with Ridgeway.  
**Action: Sue Judge.**

The issue of accessing software for data acquisition and analysis remotely was discussed. This is a known issue which depends in part on the network. Effort will be made to improve this service.

A request was made for Diamond to provide details of the nominal value of beamtime. Trevor Rayment indicated that Diamond would look into the feasibility of doing this, although was concerned about putting down a number in £, when the cost is not well defined.  
**Action: Trevor Rayment.**

It was requested that analytical methods other than OPUS to be made accessible. It was confirmed that other analytical methods such as Unscrambler are already available. Furthermore, it is possible to convert OPUS files to other formats.

The new UAS system sends automated messages to users, however once dealt with the messages should stop. Sue agreed to review to make sure this was happening.

**Action: Sue Judge**

### 12.3 Materials

The Village representatives had asked the Materials Village user community specifically for comments on Dawn. Most comments were positive, and users felt that “The introduction of DAWN was extremely useful, allowing us to make decisions and judgment about the experiment which would have otherwise been impossible. Our results are much better as a result.”

There were also positive comments about the support from the beamline staff.

There was a suggestion about the possibility of getting the Industrial Diamond group more involved with the academic organisation (one booking group?) which may help in connecting academics with industrialists or vice versa. Also, Post-experiment help for industrial users was sought. Diamond confirmed that both these tasks are already progressed by the Industrial group.

Another suggestion was to have a provision for short/quick scoping/proof-of-principle experiments that do not have to wait months for approvals from the reviewing bodies. Diamond confirmed that Rapid-access is available on several beamlines which can be made use of for such needs.

Another suggestion: the control room should try to give more information about beam dumps as estimates even such as "probably more than an hour" can aid substantially with planning sleeping patterns etc. Diamond confirmed that the Control room has been requested to provide more regular updates.

There were several comments seeking improvement in the accommodation availability in the Ridgeway Guest House and the inconvenience caused by staying off-site.

All user comments were discussed. These have been forwarded on to the relevant people on the beamlines for communication or specific responses made to some by the reps.

### 12.4 Engineering

There were a number of beamline specific comments which will be fed back to the relevant PBS, and other issues that are in hand.

Following the recent shutdown due to the RF cavity failure, the policy for users that have lost beamtime is to reapply. There was some discussion that this might not be the way to get the best science done e.g. for students. Diamond was asked to reconsider this process, and also to communicate the logic behind the decision.

**Action: Trevor Rayment & Dave Stuart**

The SLS has a time from submitting a proposal to actually carrying out an experiment of 4 months, whereas Diamond is nearer 9 months. It was agreed that Diamond would review the timescales for the process from proposal to beamtime.

**Action: Trevor Rayment & Dave Stuart**

## 12.5 Spectroscopy

The spectroscopy village received feedback from 5 member of the community. Three of these items related to the status of I20. There is ongoing concern about when I20 will be fully operational, with two members significantly concerned about the impact on the nuclear research and development programme. It was agreed in the feedback session that other ways to communicate the status of the beamline to the user community would be investigated.

**Action: Trevor Rayment**

The other responses involved aspects of the peer review process. We had one new user who was concerned about the lack of guidance in the comments from the PRP. The consensus was that new users who need assistance in preparing their initial proposals should liaise closely with the appropriate principal beamline scientist.

## 12.6 Surfaces & Interfaces

As raised in another village discussion, a user would like the value of beam time awarded to be indicated on beam time award letter. The motivation for this request is that it may help some institutions realise the value of beam time, and so aid with promotion etc, see action 11.7.

It was asked if out-of-hours support could be increased for some more complex experiments (e.g. PEEM and SXRD). Chris Nicklin indicated that it is down to each beam line how they manage their beam time support. However, if a user is concerned about support potentially being insufficient, they should contact the PBS before a beam time to discuss. It was suggested that improved manuals/training may help. Trevor Rayment indicated that a significant increase in out-of-hours support would entail recruiting more staff for this purpose, which is highly unlikely due to cost implications.

A concern was raised about the adequacy of the procedures dealing with the integrity of the technical assessment by a PBS as part of the beam-time proposal review process. The user has also questioned adequacy/speed of the complaints procedure, and the fact that any complaints were dealt with internally at Diamond. (N.B. a similar comment was made by the same user prior to the last DUC meeting.)

Trevor Rayment presented details of the peer review process, and indicated that this information was now available on the web pages for users (an action taken following the last DUC meeting). This information will be reviewed to check if clarity could be improved further. Trevor confirmed that the technical assessment will be communicated directly to the PIs. Also that if the PBSs have any concerns about the feasibility of an expt, they will contact the user in advance of the PRP.

The process states that any queries following award of beamtime are collated by the User Office and sent to the Chair of that panel for comment. These are then considered by the Science Director and a communication of the response sent to the PI.

In the event that the PI is not satisfied, the following actions will be taken. The query will be considered by the Science Director not directly involved. Diamond will seek advice from other facilities if this is required. In this case the decision of the CEO of Diamond will be final.

At the next meeting, Diamond will give the DUC a review on the outcome of the next Peer Review Process. **Action: Trevor Rayment and Dave Stuart**

It was commented that the Vending machines do not always work with the canteen cards, and it was requested if a change machine could be installed?

Sue confirmed that action would be taken to ensure that the vending machines are being regularly checked (as they should be). The possibility of installing a change machine will be looked into. **Action: Sue Judge**

There were 3 users asking for the appropriate meat in restaurant to be Halal. Sue agreed to talk to the restaurant about this. **Action: Sue Judge**

### **13. AOB**

Membership of the DUC was discussed, as 4 representatives have served their term. Dave Lawson still has 1 year to run as Chair of the committee, and so his term will be extended to 4 years. Dave then thanked Josep Sule Suso, Peter Lee and David Dye for representing the User community on the DUC.

As a result, an election will need to be held for 3 new members. **Action: Kathryn Poulter**

The next meetings of the DUC will be in March and Sept 2015. **Action: Kathryn Poulter**



**Annex A: New Actions**

<b>Number</b>	<b>Action</b>	<b>Actionee</b>	<b>Target Completion Date / Status</b>
8.2	Diamond will consider how best to move forward regarding sending outlook appointments with beamtime allocations. An update will be provided at the next DUC.	<b>B Pulford</b>	Next meeting
8.13	To make the data backup documentation from the MX webpages more widely available on the web.	<b>B Pulford</b>	Dec-14
8.13part 2	Diamond is still looking to improve external network connections and is working with STFC on this. An update will be provided at the next DUC.	<b>B Pulford</b>	Next meeting
8.13	To clarify the internal processes to encourage multi-disciplinary applications for beamtime, and how beamtime is allocated by different panels.	<b>M Walsh</b>	Next meeting
10.3	To circulate the link to the PRP process on the website to the DUC for comment.	<b>S Judge</b>	Jan-15
11.1	Trevor reported that a brochure has been published to promote the success of transactional access which he will circulate.	<b>T Rayment</b>	Dec-14
11.2	Trevor and Dave agreed to review the process regarding how Diamond responds to end of expt form feedback, and agree in consultation with Dave Lawson how this can best be used by the DUC	<b>T Rayment &amp; D Stuart</b>	Next meeting
11.3	Diamond will review procedures for hard drive tracking and report at the next meeting.	<b>D Hall</b>	Next meeting
11.4	Diamond to review whether the rotation axis function should be greyed out or password protected.	<b>D Hall</b>	Next meeting
11.5	Diamond to consider running more BAG training (as this is oversubscribed), to review the guidelines for remote users and to consider producing an online video of the "ideal data collection session" for training purposes.	<b>D Hall</b>	Next meeting
11.6	It was agreed that the User Office would discuss Late checkout as the default with Ridgeway.	<b>S Judge</b>	Next meeting
11.7	Diamond to look at whether details can be provided of the nominal value of beamtime	<b>T Rayment</b>	Next meeting
11.8	To review that the automated messages from UAS are stopped once the issue is dealt with.	<b>S Judge</b>	Dec-14
11.9	To reconsider the policy regarding cancelled beamtime after a facility wide loss of beam.	<b>T Rayment &amp; D Stuart</b>	Next meeting
11.10	To review the time from proposal submission to beamtime.	<b>T Rayment &amp; D Stuart</b>	Next meeting
11.11	To investigate other ways to provide regular feedback to the users community regarding I20.	<b>T Rayment</b>	Next meeting
11.12	To report to the DUC on the outcome of the next PRP process	<b>T Rayment &amp; D Stuart</b>	Next meeting
11.13	To review the performance of the vending machines and investigate a change machine	<b>S Judge</b>	Next meeting
11.14	To request the appropriate meat in the restaurant to be halal.	<b>S Judge</b>	Next meeting

**DUC**



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11.15	To organise an election for 3 new DUC members	<b>K Poulter</b>	Next meeting
11.16	To confirm the next meeting dates	<b>K Poulter</b>	Dec-14

**Annex B: Completed Actions**

Number	Action	Actionee	Status
6.8	Update on SCM labs at the next meeting	<b>G Cinque</b>	Most of the labs have been moved to the portacabins between zone 1 & 2 except for the Mechanical Workshop. From a user point of view the labs are accessible.
8.2	To report to the next meeting on plans for sending outlook appointments with beamtime allocations.	<b>B Pulford</b>	Will be added to the list of requirements (backlog) for the User Administration System.
8.13	To clarify the data backup process and improve documentation.	<b>B Pulford</b>	<a href="http://www.diamond.ac.uk/Beamlines/Mx/I04-1/I04-1-Manual/Data-Backup.html">http://www.diamond.ac.uk/Beamlines/Mx/I04-1/I04-1-Manual/Data-Backup.html</a>
8.14	To clarify the internal processes to encourage multi-disciplinary applications for beamtime, and how beamtime is allocated by different panels.	<b>M Walsh</b>	Next meeting
9.4	Review content and location of the Detector Group Webpages.	<b>A Dent</b>	The list of detectors presented at the last meeting will be put on the web. Action Closed.
10.1	Dave to circulate a link to the ESUO website once it is updated.	<b>D Lawson</b>	Unfortunately the ESUO website has still not been updated
10.2	Cecilia to provide contact details for the NUFO (National User Facilities organisation) in the US	<b>C Sanchez-Hanke</b>	Complete
10.3	Diamond to outline more details of the Peer Review process on the website.	<b>S Judge</b>	<a href="http://www.diamond.ac.uk/Users/UserGuide/Proposals.html">http://www.diamond.ac.uk/Users/UserGuide/Proposals.html</a>
10.4	To update on the performance of the I16 diffractometer regarding sphere of confusion.	<b>K Sawhney</b>	Yes, the sphere error is larger than a small diffractometer. We have two relevant developments: 1. An active sample adjustment based on a look-up table (on-going) and 2: A microdiffraction stage for the sample (at the proposal stage). The latter will not be available with the cryostats as they all cause very large sphere errors, but it would work with gas-jet coolers

10.5	To review Cryogenic provision on I19 and update on data handling	<b>K Sawhney</b>	<p>I19 operate, as a matter of routine, with cryostream nitrogen open-flow devices which can achieve 90 K. We have no issues with icing on the samples and these are ideal for most studies including diffuse scattering experiments where the scattering between the Bragg peaks occurs above 90 K. For temperatures down to 30 K we can use the Helix open-flow system which is also reliable and doesn't suffer from sample icing. It gets quite difficult below this temperature as the cryocool LHe system, which has a stated minimum temperature of 5K, is not as reliable as the other open-flow systems and it's very difficult to avoid sample icing. Certainly it would be difficult to carry out diffuse scattering studies as these need diffraction images free of any parasitic scattering. A closed-cycle cryostat would easily achieve the required temperatures but the scattering from the vacuum shrouds would make a diffuse scattering study next to impossible.</p> <p>The EH1 diffractometer software is Windows based and the data directory structure is somewhat unconventional. We expect that the upgrade will improve remote access to data as the data handling will then fall with the Diamond Linux infrastructure.</p>
10.6	To review user comments regarding software with the I13 beamline.	<b>P Lee</b>	Peter confirmed he had spoken with the user and PBS. Action closed.

10.7	To report on improvements to sample changer reliability.	<b>D Hall</b>	<p>For the irelec systems there have been faults with air lines (wear and tear) which have been fixed, some icing issues with lids which are being addressed by additional heating systems and the phase separator being activated.</p> <p>For the rigaku systems the dewar lids have degraded creating cold spots and consequently icing problems resulting in e-stops of the robot arm. This shutdown has seen the refurbishment of the worst dewars and all will be fixed asap. Extra heating is being added also. Other items shown as robot problems have been motor faults on the end-station – some motors have had problems but these have been fixed.</p> <p>For all cases the feedback in GDA usually implies it is a robot fault at the high level warning and it requires a little digging around to find the real cause. We will look into more explicit high level warnings explaining which error has stopped the sample exchange. Finally one of the biggest causes of failures is the use of non-SPINE standard pins. The robots are designed to use SPINE standard and it has been a requirement for users to use these since the beamlines opened. However we do keep seeing the wrong pin types. Not only do they cause problems with robot loading, some also damage goniometry.</p>
10.8	To investigate the cause of the slowdown of the GDA client during remote collection.	<b>D Hall</b>	Dave reported that we are now running on a new NX client, and will see how this performs in the next run.
10.9	To consider adding a DLS launcher to facilitate the browsing of external media connected to the Data Dispenser.	<b>B Pulford</b>	Improvements of the data dispenser are ongoing, and documentation is also being updated.
10.10	To provide an update on BioSAXS on B21 regarding what is available, and what support will be provided for data acquisition and analysis.	<b>D Stuart</b>	This was provided in Dave Stuart's presentation.
10.11	To review the approach to getting feedback from users for discussion at the DUC.	<b>D Lawson.</b>	This was discussed under item 5 on the agenda