

MINUTES OF MEETING

Title/Subject: Diamond User Committee Meeting #10

Venue:

Diamond House, G53/4

Chairman:

Dr David Lawson

Time/Date:

Tuesday 18th March 2014

Secretary:

Kathryn Poulter

PARTICIPANTS

ADDITIONAL DISTRIBUTION

DUC members

Alan Dunbar
Tom Hase
David Lawson (Chair)
Peter Lee
Rob Lindsay
John McGeehan
Feodor Ogrin
Peter Wells

Institution

University of Sheffield
University of Warwick
John Innes Centre
University of Manchester
University of Manchester
University of Portsmouth
University of Exeter
Research Complex at Harwell

**Diamond Light Source
representatives:**

Alun Ashton
Sarah Bucknall
Gianfelice Cinque
Andy Dent
Michael Drakopoulos
Paul Gibbons
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

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Apologies: Liane Benning David Dye Josep Sulé-Suso Joe Hriljac	University of Leeds Imperial College London Keele University University of Birmingham	

1. INTRODUCTIONS AND OPENING REMARKS

Dave Lawson welcomed everyone to the meeting, in particular the new representatives Alan Dunbar (Soft condensed matter), Tom Hase (Materials), Feodor Ogrin (Surfaces & Interfaces) and Peter Wells (Spectroscopy) and new Diamond staff Cecilia Sanchez-Hanke. Apologies were received from David Dye, Joe Hriljac, Josep Sulé-Suso and Liane Benning.

2. MINUTES AND ACTIONS

The Minutes of the meeting held on 24th September 2013 were approved.

Action: 6.8 – The SCM village labs & workshop will be moved during shutdowns, starting from next June dependant on the timescale of construction of I21. The mechanical workshop will be partially moved into portable cabins. An update will be given at the next DUC.

Action 8.2 – to investigate sending outlook appointments with beamtime allocations is ongoing. More discussion with DUC members is required to agree the priority, and to identify some users who would be willing to trial this email appointments system – Leave open.

Action 8.13 – Details of the data backup options available to users will be published on the new Diamond Website. The firewall is due to be changed on the 20th March. An update will be provided at the next DUC.

Action 8.14 – Clarification of the process for multi disciplinary applications is moving forward and an update will be provided at the next DUC.

Action 9.2 – Diamond policy with respect to management of data collected by diamond users will be published presently on the new web pages. It is planned that the new UAS will serve as a central interface for user notifications and actions.

The guidelines set out and distributed by Diamond user office continue to be 30 days on spinning disk. The policy clarifies that Diamond will make a single archive copy of the data but that users are ultimately responsible for the storage of data.

Action 9.4 – Andy Dent showed slides detailing the range and availability of Detectors at Diamond. The detector group have their own webpages, and the content will be reviewed.

All other actions were completed.

3. HEALTH & SAFETY

There were no issues raised.

4. ESUO

Dave Lawson attended the 6th ESUO meeting at Soleil, see Annex C for summary notes. Mike Hough (University of Essex) and Tom Hase also attended. The main purpose of this meeting was to try and formulate support through Horizon 2020. The first Horizon 2020 call will not accept proposals for Transnational access. So a continuation of BioStruct-X-like and CALIPSO-like schemes seems unlikely. Going forward, the ESUO will aim to increase its visibility, and a series of actions have been agreed. One of the key areas is to bring the website up to date. Once this is complete a link should be circulated to the DUC.

Action: Dave Lawson.

Cecilia agreed to provide contact details for the NUFO in the US for collaboration.

Action: Cecilia Sanchez-Hanke

Keith Wilson has agreed to take on the vacant role on the ESUO Executive committee. The next meeting will be in November at Max-Lab in Lund.

5. MACHINE UPDATE REPORT

Richard Walker gave a presentation to update the DUC on developments and performance of the machine.

6. PHYSICAL SCIENCES REPORT

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

7. LIFE SCIENCES UPDATE

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

8. USER OFFICE REPORT

Sue Judge gave an update on the User Office.

Peter Lee raised the issue of rooms at Ridgeway House and whether we can look at pre-allocating rooms? Sue replied that if users are able to indicate to the User office which people are on the night shift, then this could be managed.

9. SOFTWARE REPORT

Alun Ashton gave a presentation on the developments in Data Analysis.

Tom Hase asked whether the Help files continue to be updated and can anyone access them externally? Alun replied that most of the documentation from data analysis group is available outside Diamond though some beamline specific documentation may not. The help files are used in tutorials and as part of the testing for a release so there is an active effort to keep the documentation is up to date.

10. COMMUNICATIONS UPDATE

Sarah Bucknall and Silvana Westbury gave an update from the Communications group.

The new website was launched in February, and should prove better when viewing from smartphones and tablets. If anyone has any feedback, please send to Sarah and thank you to those who have done so already.

The Young Investigator award will be launched in April, with the winner being presented at the September User meeting

A new initiative called the Diamond Medal for early career research is being developed with the Royal Society and Wellcome Trust.

The User Meeting will be on the 3rd & 4th Sept, and starts at 11.00am following feedback from the last meeting. Streaming of talks from the meeting will be piloted internally this year.

There will be an IR training workshop in November as opposed to being part of the user meeting.

11. FEEDBACK FROM VILLAGE COORDINATOR BREAKOUT SESSIONS

i) Surfaces and Interfaces

User Comment (2 users):

Users wanted to congratulate Tien-Lin and his team for all their efforts to get I09 running so well.

Feedback:

Chris Nicklin indicated that he would pass on this positive feedback.

User Comment (2 users):

There was concern expressed about the lack of transparency in the peer review process of beam time proposals.

Feedback:

More details of the peer review process will be outlined on the web pages, so that it is clearer to all users, including information about how to appeal a decision. **Action: Sue Judge**

It was stated that a Principal Beamline Scientist should only review the technical feasibility of a beam time proposal. Users who have specific concerns can contact the User Office and/or the Science Directors, who will respond. Rob and Feodor were going to contact the two users,

who submitted these comments, to clarify matters further, and try to address their specific concerns.

Discussion arising from matters raised at DUC

Nexus file format for data:

It was announced that the change to the Nexus type data files is going ahead. Assurance is needed that members of the Surface and Interfaces community would be supported in terms of translators to more generic file formats or loaders for the Nexus files. Chris Nicklin indicated that such support would be provided.

ii) Materials

Everyone was complimentary about the beamline staff. 3 areas where most comments lay were: software, environmental stages/in situ and more user feedback into these.

One comment on I16 was that the diffractometer is showing signs of age. The sphere of confusion is about a factor of 10 worse than a commercial diffractometer, and this prevents a number of very nice experiments from being successful (especially with focussing on small crystals). Kawal agreed to follow up. **Action: Kawal Sawhney.**

On I19 there were a number of comments saying cryogenic provisions were not sufficient. There were comments about data handling / management side as well. Data exchange between the diffractometer is often slow. Kawal agreed to follow up. **Action: Kawal Sawhney.**

On I13 it was felt that software changes had not addressed as much of the user feedback as would have liked. It has become more difficult to use the GDA command line. Peter agreed to follow up on these specific user comments. **Action: Peter Lee.**

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

iii) Engineering

No feedback.

iv) Soft Condensed Matter

All the users who provided feedback included very favourable comments with regard to the help provided by the beamline scientists and support staff. Comments such as 'the support has been great and the beamline is working well.' were typical. There were only a few concerns raised in the users' feedback which were discussed in turn and the outcome from that discussion is provided here.

One user commented that the computers in B22 cabins were not all running the same version of the required software and some of the computers were running very slow. The village coordinator confirmed that steps are now being taken to upgrade all the computers to Windows 7 which will mean that they are all capable of running the required software. Specifically, this user group benefitted from using the data analysis room PCs and successfully carried on pre-analysis of the data. Furthermore, the software provided an estimate of the data acquisition time which was very inaccurate, leading users to think that the computers were running slower than they ought to be. This timescale estimate will be corrected once all the computers are upgraded to Windows 7.

A second B22 user commented that they received 'Absolutely fabulous support by beam line staff with all requests regarding if sample preparation, hardware or software or data analysis issues. They should be commended for dedication and willingness to try new ways with difficult samples.' The main concern of this user was that the beamline should be given more time continuously for commissioning so that they can develop and optimise difficult experimental setups. The outcome of the discussion at the DUC on this point was that in the Diamond framework each beamline has 10% of the time available for commissioning, which the PBS manages in order to address technical aspects related to the feasibility of proposals.

A further comment was made regarding noise levels in Ridgeway House, in particular loud conversations between the cleaning staff whilst occupants were trying to sleep during the day. This comment was to be passed on by the user office to the Ridgeway House management team.

Another user commented that the DAWN azimuthal integration in SAXS does not work correctly. The radial (cake) integration works fine but the azimuthal integration does not. It just gives a lot of vertical lines on the screen, however, by scrolling to the far bottom of the output there was something sensible but it is not usable. The user suggested it may be a plotting issue or an integration issue.

This user also enquired if it is possible to set up a computer at their home institution that can be used to run DAWN software and pick up any updates and/or upgrades automatically?

Finally, one user requested confirmation of what was going to happen to their allocated beamtime that was cancelled at short notice for urgent maintenance of I22. They currently do not know if this will be rescheduled and if so when.

The latter three comments are in the process of being followed up by the I22 PBS.

v) Macromolecular Crystallography MX

A number of user comments were extremely positive about the way Diamond operates, the quality and speed of data collection, remote data collection and the support from beamline personnel.

The question was asked when dewar shipping using the Diamond account would be reinstated. The issues surrounding shipping to Diamond (on the Diamond account) have now been resolved. Full instructions are here:

http://www.diamond.ac.uk/Beamlines/Mx/Common/Common-Manual/Shipping-Samples/Shipping_to_Diamond.html

Sample changer reliability was raised in discussion. The Rigaku robots (I02, I03 and I04) are very reliable, but there are recurrent issues with the CATS robots (I04-1 and I24). We are continually striving to improve the reliability of the latter. Towards this goal, the robots will be transferred to the EPICS beamline control system. This should provide useful feedback on robot performance that may help us to understand and hopefully resolve any problems. An update will be provided at the next meeting. **Action: Dave Hall**

A number of specific comments on the GDA software were made which will be investigated and planned into the GDA upgrade programme as appropriate.

One user commented that the new GDA client can be slow during remote collection. This has been reported by other users and investigations into the cause are ongoing. An update will be provided at the next meeting. **Action: Dave Hall**

It was asked whether it is possible to see what directories/files the Data Dispenser has backed up. This is currently not possible through the interface, although it will report a summary of what is on the disk in terms of numbers of files and the space used. However, it is possible to use a standard file browser (nautilus) to see what's on any of the removable disks that have been plugged into the Data Dispenser. To make things simpler for the user, we will consider adding a DLS launcher to facilitate the browsing of external media connected to the Data Dispenser. An update will be provided at the next meeting. **Action: Bill Pulford.**

The topic of BioSAXS on B21 was also discussed. It is clear that this is rapidly evolving and it would be helpful for users to get a picture of what is available, and what support will be provided for data acquisition and analysis. Now that the beamline has taken a number of users in the optimisation phase, feedback has been requested from these users to help improve the user experience going forward. Dave Stuart will summarise the situation in his Life Sciences presentation (next DUC meeting). **Action: Dave Stuart**

vi) Spectroscopy

The spectroscopy village received feedback from 6 members of the community, with the majority praising the excellence of Diamond staff and the support they received. There were a couple of comments received about Ridgeway House being fully booked, which was raised in the general discussion, specifically with regards to members of experimental teams performing night shifts. In general the comments received focussed on the peripheral needs of the user community; accommodation, food services, and online forms. The lack of feedback was discussed in the breakout session, specifically with regards to beamline development. In the breakout session it was felt that there needed to be a more proactive approach to engaging with the user community, with a more targeted effort with regards to feedback. There was a consensus that the engagement of the user community should aid in driving the science agenda of the beamlines. The suggestion of this more focussed approach to getting feedback from the user community was then raised in the general discussion and warmly received. A way forward needs to be agreed. **Action: Dave Lawson.**

13. AOB

The next meeting of the DUC will be on 23rd Sept 2014.

Annex A: New Actions

Number	Action	Actionee	Target Completion Date / Status
6.8	Update on SCM labs at the next meeting	G Cinque	Next meeting
8.2	To report to the next meeting on plans for sending outlook appointments with beamtime allocations.	B Pulford	Next meeting
8.13	To clarify the data backup process and improve documentation.	B Pulford	Next meeting
8.14	To clarify the internal processes to encourage multi disciplinary applications for beamtime, and how beamtime is allocated by different panels.	M Walsh	Next meeting
9.4	Review content and location of the Detector Group Webpages.	A Dent	Next meeting
10.1	Dave to circulate a link to the ESUO website once it is updated.	D Lawson	Next meeting
10.2	Cecilia to provide contact details for the NUFO (National User Facilities organisation) in the US	C Sanchez-Hanke	End May
10.3	Diamond to outline more details of the Peer Review process on the website.	S Judge	End June
10.4	To update on the performance of the I16 diffractometer regarding sphere of confusion.	K Sawhney	Next meeting
10.5	To review Cryogenic provision on I19 and update on data handling	K Sawhney	Next meeting
10.6	To review user comments regarding software with the I13 beamline.	P Lee	Next meeting
10.7	To report on improvements to sample changer reliability.	D Hall	Next meeting
10.8	To investigate the cause of the slowdown of the GDA client during remote collection.	D Hall	Next meeting
10.9	To consider adding a DLS launcher to facilitate the browsing of external media connected to the Data Dispenser.	B Pulford	Next meeting
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.	D Stuart	Next meeting
10.11	To review the approach to getting feedback from users for discussion at the DUC.	D Lawson.	July

Annex B: Completed Actions

Number	Action	Actionee	Status
6.8	To circulate a plan for the Soft Condensed Matter village labs, and request input from the user community	Nick Terrill/ Gianfelice Cinque	Slides in Dave Stuart's presentation about the new labs and portacabins
7.6	To clarify the process for Dewar shipping.	Dave Hall	Dewar shipping from Diamond is resolved now and is bookable against Diamond DHL account. We are working on being able to ship into Diamond.
8.2	To report to the next meeting on plans for sending outlook appointments with beamtime allocations.	Bill Pulford/ Sue Judge	Preliminary discussion on going.
8.13	To clarify the data backup process and improve documentation.	Bill Pulford	Update at next DUC.
8.14	To clarify the internal processes to encourage multi disciplinary applications for beamtime, and how beamtime is allocated by different panels.	Martin Walsh	Update at next DUC.
9.1	To send suggestion for other members for the ESUO to Dave Lawson.	All	Done
9.2	To improve the clarity of communication regarding how long data is stored for, before being archived. Including whether an email can be sent to users a week before data is archived?	Bill Pulford	Policy is due to go on the website shortly. Exp data is owned by those who do experiments. Data stored for a minimum of 30 days with at least one copy on hard disc. Users are responsible for long term storage.
9.3	To ensure that end of experiment feedback form are sent to the relevant beamline staff quickly.	Bill Pulford	Complete
9.4	To develop a list of detectors that are available at DLS and which beamline they can be used on.	Andy Dent	Andy Dent showed slides giving a summary during the meeting.
9.5	To circulate the website link to the list of offline lab eqpt that is available at Diamond for users.	Andy Dent	http://www.diamond.ac.uk/Science/Other-facilities/Offline.html Complete

9.6	To circulate a report with information on previous workshop titles, for DUC members to return ideas.	Sarah Bucknall	Complete
9.7	To investigate live streaming of the SR user meeting and offering the IR training online.	Isabelle Boscaro-Clarke	Will be piloted internally this year. Further info in Comms update
9.8	To suggest names for the early career award to Isabelle.	DUC	Further info in Comms update
9.9	To issue a revised proposal for the Young Investigator award.	Isabelle Boscaro-Clarke	Further info in Comms update.
9.10	To investigate holding the workshop on IR data analysis on a yearly basis.	Gianfelice Cinque	This is provisionally booked w/s 10 Nov 2 days hands on training by CAMO.
9.11	To write a simple summary of the benefits of moving to Nexus for discussion.	Paul Gibbons	Physical Science beamlines will move to Nexus.
9.12	To inform users regarding the location of the instructions for data copying on the MX webpages.	Sue Judge/Dave Hall	Close
9.13	To organise an election for 4 new DUC members	Kathryn Poulter	Complete

Annex C

6th ESUO meeting 6th-7th March 2014 at Soleil

UK representatives:

- Dave Lawson (John Innes Centre) – DUC chair
- Mike Hough (University of Essex) – Life Sciences user of BioStruct-X
- Tom Hase (University of Warwick) – Physical Sciences user of CALIPSO (and Materials rep. on DUC)

The first HORIZON2020 call will not accept proposals that are specifically for large scale TransNational Access (TNA) activities. Thus, a continuation of BioStruct-X-like and CALIPSO-like schemes seems unlikely. Instead TNA could be supported as part of proposals addressing “Grand Challenges”. Thus, to maintain support for TNA at current levels would require a very fragmented approach through multiple applications. As an alternative, it has been proposed that TNA could be incorporated into proposals that include Joint Research Activities (JRAs), with the focus on developing equipment and methods for advanced synchrotron experiments, but driven by the users (as European consortia), not the facilities themselves. It was noted (Tassos Perrakis) that a HORIZON2020 call exists that mentions improving the availability of X-ray scattering to a wider community:

<http://ec.europa.eu/research/participants/portal/desktop/en/opportunities/h2020/topics/64-infraia-1-2014-2015.html>

Concerns from users regarding the current requirement to make in effect ‘double applications’ for beamtime and BioStruct-X support was raised, but it is unlikely that this will change before the end of the project.

The CALIPSO website <http://www.wayforlight.eu> is proceeding well and work is underway for a common beamtime application form for the facilities. Work was underway to have the ability to mark several applications as complementary to help with scheduling.

In November 2013, Ulli Pietsch (chair of ESUO) sent a “letter of concern” to the European Commission on behalf of ESUO outlining our concerns regarding TNA (attached). He has not received any response so far.

Going forward it was proposed that ESUO should go on a “lobbying offensive” over the coming year in order to improve ESUO visibility and emphasise the value of TNA, towards influencing the priorities for the next HORIZON2020 call. The following specific actions were proposed:

- Submit letters of concern to *J. Synch. Rad.* and *Nature*.
- Prepare a small brochure focussing on the socio-economic impact of TNA as material for lobbying program committees and other political bodies.
- Attending lobbying events such as European Parliament breakfast debates.
- Improve/update the ESUO website.
- Advertise importance of TNA/ESUO through presentations/posters at facility user meetings and on facility websites.
- ESUO to arrange a European Synchrotron Users Conference to facilitate the exchange of ideas towards the preparation of JRA-based applications to HORIZON2020.

Keith Wilson (University of York) sits on the Project Evaluation Committee of BioStruct-X and was proposed as suitable candidate for a vacancy on the ESUO Executive Committee. He has subsequently agreed to take on this role and, by default, will also serve as an ordinary member of ESUO (the 4th UK representative!).

Next meeting proposed for November 2014 at MAX-lab in Lund.

Dave Lawson (13th March 2014)