

MINUTES OF MEETING

Title/Subject: Diamond User Committee Meeting #9

Venue: Diamond House, G59

Chairman:
Prof. Bill Clegg

Time/Date: Tuesday 24th September 2013

Secretary:
Kathryn Poulter

PARTICIPANTS

ADDITIONAL DISTRIBUTION

DUC members

Liane Benning
 Bill Clegg (Chair)
 David Dye
 Karen Edler
 Joe Hriljac
 Karen Hudson-Edwards
 David Lawson (Chair)
 Peter Lee
 Rob Lindsay
 John McGeehan
 Josep Sulé-Suso

**Diamond Light Source
representatives:**

Isabelle Boscaro-Clarke
 Sarah Boundy
 Gianfelice Cinque
 Andy Dent
 Michael Drakopoulos
 Paul Gibbons
 Dave Hall
 Susan Judge
 Burkhard Kaulich
 Chris Nicklin
 Kathryn Poulter
 Bill Pulford
 Trevor Rayment
 Kawal Sawhney
 Dave Stuart
 Richard Walker
 Martin Walsh
 Jorg Zegenhagen

Apologies:

Keith Meek

Institution

University of Leeds
 University of Newcastle
 Imperial College London
 University of Bath
 University of Birmingham
 Birkbeck College
 John Innes Centre
 University of Manchester
 University of Manchester
 University of Portsmouth
 Keele University

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

University of Cardiff

1. INTRODUCTIONS AND OPENING REMARKS

Bill Clegg welcomed everyone to the meeting, in particular the new Spectroscopy village representative Liane Benning, and new Diamond staff Jorg Zegenhagen (Experimental co-ordinator) and Sarah McBean (Science division PA).

Apologies were received from Keith Meek

2. MINUTES AND ACTIONS

The Minutes of the meeting held on 5th March 2013 were approved.

Action 8.2 to investigate sending outlook appointments with beamtime allocations is ongoing. The technology is available, however more discussion with users/user office is needed to agree use cases for implementation. Dave Lawson volunteered to be involved.

Action 8.13 to clarify the process of data backup is ongoing. Discussion then followed on data archiving and what Users wanted to be able to do i.e. take their data away with them or via FTP over the network. David Dye asked how frequently Users asked to access archived data. Whilst Diamond's published policy is to keep archived data for 180 days, data will in fact be kept on tape for the lifetime of the storage medium.

Action 8.14 regarding multi-disciplinary applications for beamtime is ongoing. The intention is to implement processes in the new User Administration system to avoid double applications. Additionally MX BAGS are being encouraged to put SAXS and CD time into their beamtime applications. The BioSAXS beamline is expected to be online shortly.

All other actions were completed.

3. HEALTH & SAFETY

There were no issues raised.

At this point Bill handed over as Chair to Dave Lawson.

4. ESUO

Dave Lawson attended the 5th meeting 19-20th Sept at SLS, see Annex C for summary notes. There was discussion at the meeting regarding increasing the visibility of the ESUO. Some of the actions agreed included increasing the UK delegates to 3, presenting ESUO activities at the SRUM and preparing a case for Horizon 2020. The next ESUO meeting will be held in March 2014.

Some discussion followed on how these organisations interact with Diamond. Trevor replied that Diamond is really keen that there should be no barriers to people coming here from

overseas. Dave Stuart added that it is important for Diamond to encourage more international scientists via transnational access.

There was discussion regarding the merits of a UK national synchrotron users group, however it was felt this was not the best way forward. A mechanism is needed for selecting more UK-based reps for the ESUO. DUC members were requested to send suggestions to Dave Lawson.

Action: All

5. USER REPRESENTATIVES REPORT

i) MX

Overall feedback from the users was extremely positive.

- 1) There had been an enquiry regarding requesting short shifts. Dave Hall replied that users were encouraged to talk to the relevant beamline scientist regarding scheduling
- 2) From AP14, users can specify how much remote access vs onsite time they have.
- 3) There have been some small problems with returning dewars. This system is currently under review.
- 4) Unipuck system can be requested in advance of beamtime, and if a spare system is available it will be provided on loan.
- 5) It was requested that Diamond improve the clarity of communication regarding how long data are stored for, before being archived. Can an email be sent to users a week before data is archived?
Action: Bill Pulford
- 6) During remote access, there have been issues with data not being backed up to the hard drive supplied by the users. Dave Hall replied that Diamond plugs the hard drive in, but it is the user's responsibility to initiate the backup process.
- 7) There have been mixed views on the new GDA, however in general it was felt to be improving every visit.
- 8) A point was raised regarding who received the end of experiment feedback form. There was an expectation that it was sent to the local contact. Dave Stuart replied that this issue had been raised at the last BOCC Meeting and there was an action on Bill to come up with a way to distribute it back to the relevant people on the beamline quickly.

Action: Bill Pulford.

ii) Soft condensed matter

- 1) One user had problems using the DAWN software, a) following the help videos as these vary from version to version, and b) downloading the new version. The I22 beamline staff are in the process of taking over the help files with the aim to make them more user friendly. The problems related to changing versions are a known bug and Diamond is aware and working on it.
- 2) It was asked if there was a plan to have a permanent beamline suitable for protein SAXS? The existing plan is to have B21 for high throughput SAXS including BioSAXS giving a more stable platform for this group of users.
- 3) There was one comment regarding the misalignment of the beam on I22. This will be resolved by the I22 team directly.

iii) Materials

In general the feedback was very positive. Direct comments have been sent to the relevant PBS for action.

- 1) There was a request to upgrade the detector on I19. Currently there is a plan to replace EH1 which will become a high throughput station and to have EH2 running a Pilatus detector routinely.
- 2) It was noted that it was critical to have a temperature controlled sample environment for XPCS on I13C. Additionally an accurate thermometer is needed at the sample position.
- 3) There were a number of complaints about the food particularly in the evenings.

iv) Engineering

Feedback received was all from I12 users who were extremely complimentary about the beamline staff and assistance/support received. One user did have problems with data transfer both during the beam time, and then during the summer shutdown, where he felt there were frequent shutdowns and reconfiguration of the IT structure without notification to users.

One suggestion was for a better description of detectors available at DLS and which beamlines they could be used on.

Action: Andy Dent

A second comment regarded the need for working with radioactive materials, specifically depleted uranium. This is already possible, so the message has been passed on to the user. A third comment regarded some problems with long radiograph exposures at I12, and a solution is already being worked on.

v) Surfaces & Interfaces

It was asked whether people can be assigned quieter rooms at Ridgeway House, as there was a lot of noise during the day from nursery. Bill replied that this can be done if you ask in advance of arrival.

There was a request for more sample environment stages on I07. Chris replied that there is always the possibility of developing equipment to meet specific requirements if these are discussed well in advance of beamtime with the Beamline scientists.

There was a concern expressed about the lack of standard software for data reduction on I07. The beamline staff are aware of this issue and a project is in place to develop software for surface diffraction, reflectivity and small and scattering data reduction.

vi) Spectroscopy

There was a comment received on evaluation of proposals, in that the Hard and soft x-ray panels evaluate proposals differently. Trevor replied that membership of the PRP changes

frequently, and that we try to cover all areas of Science but this is not easy. Any suggestions for representatives would be appreciated.

A query was raised as to whether beamtime dates could go to the PI and CI? Sue replied that this facility was available, but the PI has to choose this option.

There was a comment that when users have beamtime split across a Tuesday, there was often a need for additional money on the cashless card. Sue replied that in this case, a user just needs to stop by the user office and this can be sorted out.

There was a request for a list of offline equipment that is available at Diamond for users. This is currently available on the website, and Andy agreed to circulate the link.

Action: Andy Dent.

It was asked if the check out time at Ridgeway could be changed from 10am to 12pm. This is currently available on request.

There is a lack of healthy snacks in the Vending machines. This is something that Sue is looking into.

6. MACHINE UPDATE REPORT

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

Peter Lee requested that there be a walkway from the cafeteria/DH through I14 to I13. Richard replied that it would be considered, however there are budget constraints for the building

7. PHYSICAL SCIENCES REPORT

Andy Dent 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.

9. USER OFFICE REPORT

Sue Judge gave an update on the User Office.

A demonstration of the new User Administration software was given. The intention is that all functionality will be available via one application with the same look and feel.

Please feedback any other requirements to Sue Judge.

10. SOFTWARE REPORT

Paul Gibbons gave a presentation regarding the earlier papers distributed regarding the use of Nexus vs ASCII files.

This generated significant discussion. In summary it was agreed that if there was to be a move to Nexus, there had to be tools in place to create ASCII files that are equivalent to the current ASCII files provided.

It was also likely that moving to Nexus would aid developers of analysis programs and hence aid the integration of the analysis with data collection.

Dave Lawson agreed that there would be no decision here today. It needs to be taken offline between the villages to discuss what the pertinent issues are.

11. SR USER MEETING

The recent user meeting was reviewed. There was a suggestion that it could start later on the first morning, which would mean finishing later on second day. Alternatively registration could be after lunch.

It was agreed that the welcome talk/registration should be before lunch.

Any suggestions for workshops and keynote speakers for the 2014 meeting would be welcome. Sarah Bucknall will circulate a report with information on previous ones, for DUC members to return ideas. Plans will then be reviewed at the March meeting. **Action: Sarah Bucknall**

Bill asked whether there were other rooms on campus that could be used so that the meeting could be extended.

Sarah replied that we already use the Research Complex. We have previously used the Electron building and HPA, however this does make these workshops more remote. Additionally the capacity of the lecture theatre is an issue. David Dye made the suggestion of live streaming of talks.

Liane asked if the IR training could be run more often than every 3 years – or if it could be offered online? Isabelle agreed to investigate both suggestions. **Action: Isabelle Boscaro-Clarke**

A document outlining the Young Investigator award was circulated in advance of the meeting. There was some discussion on the Early Career award, and where we set the upper age/experience boundary. It was agreed that the Early Career award should be for people up to 5 years after the formal announcement by an awarding body of their PhD. EU declaration on career breaks/part time working etc should be adopted.

The offer of beamtime at Diamond as a prize was suggested, however Trevor confirmed that this has previously been investigated and has been found difficult to implement,

The issue was raised that there are many Lawrence Bragg awards. Please could DUC members send any suggestions for names for the early career award to Isabelle. **Action: DUC**

A revised proposal will then be issued.

Action: Isabelle Boscaro-Clarke

12. FEEDBACK FROM VILLAGE COORDINATOR BREAKOUT SESSIONS

i) Surfaces and Interfaces

The earlier proposal to change the data file format to Nexus was discussed. It was concluded that many members of the Surface and Interfaces community would require translators to generate more generic file formats from the Nexus files, allowing them to use already developed analysis software. Other Villages suggested that this issue could easily be resolved by software providers, but such individuals/companies generally do not exist in this research area; most software development is undertaken by PhDs/PDRAs on a somewhat ad hoc basis.

ii) Materials

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.

iii) Engineering

I11 – It was commented that for High throughput low resolution diffraction, it was hard to get beamtime. Trevor stated that decisions were made on the science case presented.

I12 – Perceived as an engineering beamline rather than a high energy beamline. I12 does offer a small beam size but it is not focused.

There was some discussion regarding trying to make experiments quicker, because the beamline is oversubscribed. One way forward is for I12 to offer a unified interface to those sample environments which are used by a significant number of users.

iv) Soft Condensed Matter

Feedback on the recent workshop on IR data analysis was good, and it was requested if this could be held on a yearly basis. The workshop currently focuses on Opus, but other types of software could be included. **Action: Gianfelice Cinque**

The new I21 beamline will go through the peripheral labs of this village. Current expectation is that the affected labs and workshops will be moved to portable labs in the March/Apr -14 shutdown. The labs for the village will then be consolidated in 2014.

v) Macromolecular Crystallography MX

The issue of Nexus was discussed, and it was agreed that a simple summary of benefits is needed and consultation with the software developers. **Action: Paul Gibbons**

Some work will be undertaken shortly to make IspyB more user friendly.

Regarding Dewar shipping, Diamond is moving towards a situation where DHL handle UK shipments through a centralised contract.

Instructions for data copying are now on the MX webpages. This information needs to be communicated to users. **Action: Dave Hall /Sue Judge**

vi) Spectroscopy

There was some discussion regarding peripheral lab instrumentation, and the process for users to get access prior or post beamtime. The details for this are on the website.

It was commented that User manuals should be more available and “dummy proof” e.g., for irregular or new users. This is being actioned internally.

13. AOB

Membership of the DUC was discussed, in that turnover needs to be 4 people /year. Dave thanked Bill for steering the DUC for last 2 years, and additionally Keith Meek, Karen Edler and Karen Hudson-Edwards for representing the User community on the DUC

As a result, an election will need to be held for 4 new members. **Action: Kathryn Poulter**

The next meetings of the DUC will be in March and Sept 2014.

Annex A: New Actions

Number	Action	Actionee	Target Completion Date / 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	Next meeting
7.6	To clarify the process for Dewar shipping.	Dave Hall	Next meeting
8.2	To report to the next meeting on plans for sending outlook appointments with beamtime allocations.	Bill Pulford/ Sue Judge	Next meeting
8.13	To clarify the data backup process and improve documentation.	Bill 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.	Martin Walsh	Next meeting
9.1	To send suggestion for other members for the ESUO to Dave Lawson.	All	Next meeting
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	Next meeting
9.3	To ensure that end of experiment feedback form are sent to the relevant beamline staff quickly.	Bill Pulford	Next meeting
9.4	To develop a list of detectors that are available at DLS and which beamline they can be used on.	Andy Dent	Next meeting
9.5	To circulate the website link to the list of offline lab eqpt that is available at Diamond for users.	Andy Dent	End Dec
9.6	To circulate a report with information on previous workshop titles, for DUC members to return ideas.	Sarah Bucknall	End Nov
9.7	To investigate live streaming of the SR user meeting and offering the IR training online.	Isabelle Boscaro-Clarke	Next meeting
9.8	To suggest names for the early career award to Isabelle.	DUC	Next meeting
9.9	To issue a revised proposal for the Young Investigator award.	Isabelle Boscaro-Clarke	Next meeting
9.10	To investigate holding the workshop on IR data analysis on a yearly basis.	Gianfelice Cinque	Next meeting

9.11	To write a simple summary of the benefits of moving to Nexus for discussion.	Paul Gibbons	End Dec
9.12	To inform users regarding the location of the instructions for data copying on the MX webpages.	Sue Judge/Dave Hall	End Dec
9.13	To organise an election for 4 new DUC members	Kathryn Poulter	End Dec

Annex B: Completed Actions

Number	Action	Actionee	Status
5.4	To restructure the MX village web pages – Final release to be made in March-13.	Dave Hall	Complete
6.8	To circulate a plan for the Soft Condensed Matter village labs, and request input from the user community	Gianfelice Cinque	Nothing to present yet, action ongoing.
7.6	To clarify the process for Dewar shipping.	Dave Hall	Ongoing – not as simple as first thought. Will be discussed in the breakout session.
8.1	To consult with the DUC regarding representatives for the ESUO	Bill Clegg	Not done. Dave L went to the most recent meeting. Will be discussed under item 4.
8.2	To report to the next meeting on plans for sending outlook appointments with beamtime allocations.	Bill Pulford/ Sue Judge	Ongoing.
8.3	To request that the restaurant be able to provide “on demand” meals at the weekend.	Sue Judge	Sue reported that the Restaurant are happy to cook on request if people have specific dietary requirements.
8.4	To provide distribution lists of users to the DUC reps, so that they can be contacted for feedback in advance of the next DUC.	Sue Judge / DUC reps	Complete. Noted that this was a much more successful way of obtaining feedback and should be repeated.
8.5	To e-mail I11 users to explain the plans for bringing I11 back online in Sept-13.	Chiu Tang / Sue Judge	Complete.
8.6	To provide a distribution list for the spectroscopy village to Karen Hudson-Edwards.	Sue Judge	Complete
8.7	To report back on the summary of feedback regarding software.	Karen Hudson-Edwards	Complete

8.8	To look into providing weekend support for small machining jobs for users.	Trevor Rayment	<p>The Experimental Hall Coordinators (EHCs) are trained in basic workshop tools which means they can provide support out-of-hours (evenings/weekends) for drilling, cutting, filing etc. They have already provided this type of support to various users on several beamlines.</p> <p>They are not trained to machine materials i.e. they cannot use the lathe or the milling machine.</p>
8.9	To clarify the process of using the UHV surface eqpt in the offline lab.	Chris Nicklin / Trevor Rayment	Complete - The website has been updated.
8.10	To inform I15 users on recent changes to staff and beamline eqpt.	Heribert Wilhelm / Sue Judge	We have sent emails to I15 users since the DUC meeting to update on staffing and new equipment. Furthermore, we try to keep the webpage always up-to-date.
8.11	To make a plan for the dark period for I15 for providing beamtime for routine high pressure work, and communicate dates for the shutdown.	Heribert Wilhelm / Trevor Rayment	<p>The community will be kept up to date via email.</p> <p>Joe commented that the communication had been good.</p>
8.12	To outline the upgrades that are scheduled to be made to the Data dispenser.	Bill Pulford	Complete
8.13	To clarify the data backup process	Bill Pulford	Ongoing - Bill to improve documentation including the website, and look at increases in speed.
8.14	To clarify the internal processes to encourage multi disciplinary applications for beamtime, and how beamtime is allocated by different panels.	Martin Walsh	Ongoing.
8.15	To allow more time for the breakout session in the next agenda.	Kathryn Poulter	Complete
8.16	To investigate putting a vending machine in the restaurant.	Sue Judge	STFC are not convinced that this will work, and are looking at other options such as extending hours at weekend instead.
8.17	To include the link to the UAS in the minutes.	Kathryn Poulter	Complete

8.18	To ensure that comments can be captured to help with error messages.	Bill Pulford	Implemented via a button in GDA for comments. Alternatively by email to dascjira@diamond.ac.uk for GDA and the Data Acquisition group, to scisoftjira@diamond.ac.uk for general scientific software issues and to dawnjira@diamond.ac.uk for DAWN related issues and comments.
8.19	To clarify the conditions for entering into the Young Investigator award	Isabelle Boscaro-Clarke / Trevor Rayment	See document for discussion.
8.20	To coordinate the process for electing a new Chair of the DUC.	Kathryn Poulter	Complete

Annex C

5th ESUO meeting 19th-20th Sept 2013 at the Swiss Light Source

ESUO (European Synchrotron Users Organisation)

Established in 2010 to support Transnational Access (TNA) to European synchrotron radiation sources (and now free electron lasers)

- founded under the ELISA project (European Light Sources Activities)
- acts as a lobbying organization for extension of EU funding to transnational access based activities

Presentations

- ESUO activity report
- National User Organisations summary (compiled from delegate input):
 - 13, 000 users from 23 countries; 13 national user organisations
- Status of SLS and the SwissFEL
- Overviews of CALIPSO, BioStruct-X and Umbrella

TNA access supported under two FP7 projects:

- **CALIPSO** (Coordinated Access to Lightsources to Promote Standards and Optimization) - started June 2012
 - for physical sciences
 - single entry point (www.wayforlight.eu) to simplify access
- **BioStruct-X**
 - for life sciences
 - cooperates with the ESRFI project Instruct (Integrated Structural Biology Infrastructure for Europe) in aiming to provide an integrated and coordinated technology platform to all relevant methods in structural biology.

Umbrella is the pan-European federated identity system for the users of the European large photon/neutron facilities (<https://umbrellaid.org/euu/>)

- to provide a single access portal and project evaluation procedure
- single login enabling access to all facilities
- optimise the process from experimental data acquisition to data publication
 - data acquisition
 - data analysis
 - data transfer
 - trans-facility experiments
 - remote data access (ICAT, under development)
 - remote experiments (Moonshot, under development)
- Diamond will connect to Umbrella in November 2013 (DLS collaborates on CRISP, PaNData, CALIPSO)

ESUO plans

- Increase visibility of ESUO
- More delegates (3 for UK - has been discussed previously at DUC)
 - preferably users of other European facilities. e.g. a Physical Science rep, a Life Science rep plus the DUC chair
- ESUO presentations at facility meetings?
- Improve website (not been updated for several months)
- write a letter to EU commission concerning the importance of TNA - to be sent to *Nature* too
- Preparing a case for Horizon 2020 (see below)
- Next ESUO meeting possibly in March 2014 - venue TBA

Preparing a case for Horizon 2020 funding 2014-2020 (FP7 follow-up; €80 billion research and innovation funding programme)

- 5 working groups established from ESUO delegates:
 - Energy and resources
 - Instrumentation and standardisation
 - Life sciences and biomaterials
 - Cultural heritage and environmental and geosciences
 - Advanced materials (surfaces and interfaces) and diluted matter and soft matter
- Vision for structural biology to cover: protein production, BioNMR, X-ray, EM, HybridSB

Questions

- How do these organisations currently mesh with DLS?
 - Implications for new UAS
- What can we (DUC/UK user community) do to help?
 - ESUO presence/presentation at SRUM?
 - Should there be a national user organisation?
- Where should additional ESUO delegates come from?