From: STFC Physical Sciences and Engineering Advisory Panel

To: STFC Science Board

Cc: Dr Jennifer Scratcher, STFC Secretariat

Date: Wednesday 3rd February 2016

Feedback from Physical Sciences and Engineering Advisory Panel 2015 consultation exercise

Executive Summary

In 2015 the Physical Sciences and Engineering Advisory Panel (PS&EAP) trialled a new survey format that is intended to provide a portal by which its user cohort can readily connect to their AP on matters connected with relevant Central facility (CF) usage and capability. The intention is for (i) the survey to be open throughout the year, (ii) responses to be correlated and documented quarterly, and (iii) briefing documents to be produced bi-annually. Further, the documents summarising major aspects of the survey returns will be mounted on the PS&EAP webpages. Once active, such a portal could be used to seek feedback on particular topics as the needs arise.

The 2015 trial was reasonably successful but it did reveal certain problems. One such problem is an uneven format for how prompts for survey engagement are dispatched. The main points of the survey are described in Section 3 of this report. Moreover, on analysing the feedback, several topics came to the fore which the AP thought should be passed on to its parent body (Science Board, SB). Those matters are covered in a separate document (Issues arising from analysis of PS&EAP 2015 consultation exercise, February 2016).

The PS&EAP are well placed to actuate this form of consultation exercise in 2016, thereby fulfilling their remit to "consult and interact with the community and to ensure its views are canvassed" (PS&EAP Terms of Reference, 2014).

1. Background

The Physical Sciences and Engineering Advisory Panel (PS&EAP) Chairperson attended a Science Board (SB) meeting held at the Cockcroft Institute on Friday 27th February 2015, when he reported on PS&EAP activities that had taken place over the last 12 months. One of the items considered during that encounter was the PS&EAP's initial attempt at a consultation exercise that was conducted in the autumn of 2014. Although the number of respondents was modest, the quality of the replies was good, resulting in some useful feedback on a variety of topics relevant to Central Facility (CF) users active in the areas of Engineering and the Physical Sciences. Indeed, those interactions prompted the AP to subsequently provide SB with briefing documents on the benefits of maintaining STFC capability for (i) ISIS and the ILL as well as (ii) Diamond and the ESRF.

The 2014 consultation exercise utilised the newly instigated PS&EAP webpages (http://www.stfc.ac.uk/about-us/how-we-are-governed/advisory-boards-panels-committees/physical-sciences-and-engineering-advisory-panel/). Lessons learnt from this initial consultation concerning how the AP could sustainably achieve Remit 2.4 of the AP Terms of Reference (9/6/2014), *i.e.* "Consult and interact with the community to ensure its views are canvassed and there is an appropriate and effective route for communication with STFC on strategic programmatic issues" were broached in the February SB meeting. These discussions prompted the PS&EAP Chairperson (DL) to adjust the consultation format and to set up a trial exercise in June 2015 that was actuated in September 2015. The revised format is briefly outlined below.

Faced with the prospect of considering when to repeat an engagement exercise with the PS&E user community, DL decided to use the AP webpages to mount an open portal, which CF users could access at any time throughout the year. The PS&EAP would then arrange to review inputs on a quarterly basis and to bi-annually mount a short summary of responses received on the AP webpages. This arrangement would then mean that the AP can be readily approached by its designated user community on any subject within its jurisdiction. The AP would filter and prioritise this information and, if required, select topics for further subsequent investigation by the AP acting as an Expert Panel. In this way, it is intended that CF users will have an open conduit to the PS&EAP which, via its connections to Science Board, can inform decisions on future investments and scientific priorities that are of direct relevance to the UK scientific community.

The introductory material emphasized that this consultation only related to practitioners in Physical Sciences and Engineering and asked researchers to respond to a set of seven questions after identifying their principal area of research as defined by the following four categories: (i) Photon

Sources, (ii) Neutrons and Muons, (ii) Laser Sources and (iv) Other. On 29th September 2015 the STFC Secretariat asked the Facility Directors of Diamond, ISIS and the CLF to circulate via their respective user databases a request for researcher engagement in the AP consultation. The consultation deadline was set for 30th November 2015. Section 3 provides a summary of responses received.

The results were discussed at the PS&EAP annual meeting held in Swindon on Tuesday 19th January 2016. Here, acting as an Expert Panel, matters raised in the survey responses were reviewed and the following four distinct topics were judged to be worthy of further scrutiny: (a) concerns over sustained operational capability of ISIS and the ILL; (b) deficiencies of Diamond's provision for researchers in the Physical Sciences, (c) an understated role for engineering related research within the STFC portfolio of CFs; and (d) opportunities with high power laser systems. These matters were deemed of such importance to UK science capability that their cases are briefly outlined in a separate document – "Issues arising from analysis of PS&EAP 2015 consultation exercise".

2. House-keeping matters

The AP then went on to consider the distribution of responses received according to the four sub-divisions outlined above (Section 1). Whereas it is conceded that the overall take-up was modest, it was abruptly apparent how skewed the distribution of responses were when viewed by sector. Table 1 presents the distribution of returns.

Area of research activity	Number of responses
Photon sources	41
Neutrons and muons	17
Laser sources	2
Other areas	5
TOTAL	**65**

Table 1. Responses received for PS&EAP 2015 community consultation exercise according to respondents' principal connection to a Central Facility. These numbers indicate the total responses received; some of which were unusable.

This prompted the AP to further investigate how the consultation exercise was communicated to the CF usergroups. On 13th October 2015 Diamond distributed the PS&EAP request for engagement via a discrete circulation to all of its users. Anecdotally, it is understood that this dispatch reached a wide number of CF users. ISIS distributed the request to engage in the survey on 21st October 2015 via an ISIS Community News email. However, the dispatch had two parts and the PS&EAP

component was at the end of the message; any PS&E practitioners had first to pass over details of the IOP 2015 Magnetism Winter School at the University of York before arriving at the PS&EAP piece. It is felt highly likely that a large number of users actually missed our message and simply deleted the email. The PS&EAP have no evidence of a dispatch from the CLF. Members of the AP with connections to the CLF confirmed that they had not received any request via the CLF for engagement with the PS&EAP survey. The returns noted in Table 1 are broadly in agreement with the scenarios outlined above.

SB are asked to recall the reluctance of Facility Directors to engage with the PS&EAP 2014 consultation exercise (PS&EAP presentation to SB, 27/2/2015). *Should STFC and SB value PS&EAP's efforts to consult with its associated cohort of CF users in the manner outlined above, could those senior bodies please work out a conduit for dissemination that is acceptable to the Facility Directors (FDs) who control access to the CF user databases.* This should be done without FDs influencing the nature of the questions contained within any of the surveys; the independence of the AP is vital to its integrity as a representative body within the research community of which it seeks to serve.

The AP also needs to acknowledge that, despite prior testing by the STFC web team, several IT problems were encountered in the early stages of the survey period. These problems were subsequently overcome although some returns were thought to be lost and/or corrupted in the interim period. Furthermore, during analysis of the survey returns during the recent PS&EAP meeting in Swindon, it was noticed that no returns were recorded in the last weeks of the survey period. This again is attributed to an IT problem, which is thought to be responsible for significantly restricting the number of documentable returns (folk tend to respond near to the deadline).

2.1 A forward look to further consultation

- The STFC Secretariat is in discussions with the STFC web team to make the format of the questionnaire more durable and more amenable to post-survey processing. They will also ensure that premature terminations of the questionnaire do not reoccur.
- A sub-committee of the PS&EAP has been set up to review how the 2015 consultation exercise could be improved upon. This includes the structure of the questionnaire and the questions that it asked. The 2015 exercise covered matters connected with the local operation of a particular CF, as well as asking users how they viewed STFC's role in managing the large-scale and long-term operations. The balance and appropriateness of these questions will be re-examined.
- SB is asked whether they would want to see certain topics examined in future surveys.

3. Summary of significant points gleaned from the survey

3.1 Photon Sources (33 responses)

33 usable responses, of which ~90% (30/33) are users of Diamond, 30% (10/33) ESRF, and 4 use ISIS, 2 FEL and 1 ILL. Of the respondants, 33% where life science (mostly structural biology), and the rest PS&E, with key areas being planetary science, polymer chemistry and materials.

Capability of the Large Central Facilities (LCF's)

Almost all responses were complementary of the facilities and facility staff, with a few 'satisfactory'. The only 'inadequate' was for eBIC, but they mentioned this was new and the main suggestion was to expand it. (AP comment – eBIC is less than 25% operational, so this happening.)

There were many useful suggestions for improvements, with several flagged below.

- Do the LCF's provide state of the art capability?
- Almost all responses thought Diamond and ESRF were state of the art.
- Many recognised what one respondent summarised "es, but of course needs to be constantly monitored/improved to stay state-of-the-art". Suggestions to do this included:
- Time-resolved EXAFS would provide internationally competitive capability in basic science
- Advances are being made in fluorescence detector technology and investment in this area will be needed to maintain leadership
- My only concern is man-power. More man-power is needed to support external users
- Inferior slow CCD detector and inefficient commercial control and data processing software needs replacement, which is planned
- Data reduction and visualisation capabilites in Engineering do not match those available to the life science community, particularly Macromolecular Crystallogaphy (MX). The MX community has achieved much over the years through significant funding of software development. Similar investment is needed in the physical sciences and engineering.
- A common issue is however analysis software, particularly for real-time
- It would be good to develop submicron beamlines to rival FEL.
- (Need) hard X-ray high resolution powder diffraction

Developments over 5-10 years

A wide range of suggestions were made, but there were some core themes:

- Increased effort in automation, both hardware and software
- Improved detectors
- Improved analysis software, both for real time analysis to improve experiments on the fly, and for analysis and visualisation afterwards

Many respondents emphasised the need for continual upgrading, as well as new sources / beamlines There were a number of specific comments worth highlighting:

- removable sample chamber for the use of low-energy X-rays
- Improved access for industry with better expertise in a diverse range of areas on hand to perform and develop experiments useful to industry.
- high efficiency, high energy-resolution detector technology
- further technical developments on the detector side, i.e. in photoemission technology, with respect to better energy, momentum, and spatial resolution as well as to improvement of data acquisition efficiency
- more automated data collection and rapid access beamtime
- while the hardware of the facilities (are) important, the people who staff it make the world-leading science
- Laser-shock compression

- Simplification of the data analysis process and education in term of how to access the most appropriate data analysis software.
- X-ray tomography to produce 3D structures within thin film samples
- ancillary instrumentation available for off-line work and formalize user access to such instrumentation.
- Full off-site user access to all data processing software.
- Faster access routes (currently you apply for beam time 6months ahead of the start of a 6month period, meaning it could be up to 1year before the experiment is actually performed).
- High pressure and high temperature PDF-experiments.
- remote access and ideally "unmanned" access i.e. automatic and robust
- More permanent staff to support the overall operations
- better integration of central facilities with central high performance computing.
- Science and not-technical oriented beamlines (for example: catalysis, time-resolved physics/chemistry, extreme conditions).
- Further development/building of research centres and location of regular SR users at these 'light campuses' would surely strengthen the impact of research collaborations, particularly when performing demanding and novel experiments
- Advances in data collection and analysis software need to be made to keep up with the large volume of data being measured using faster detectors.
- in situ / in operando measurements … to understanding processes/ materials where by its nature many data sets are recorded.
- Stronger links between neutron and X-ray to make proper use of the complementarity in diffraction and spectroscopy.
- Provision of leading edge VUV/SXR light sources

3.2 Neutrons and Muons (18 respondents)

- *Does the Central Facility(ies) provide state-of-the-art capability?*

All respondents strongly agreed that ISIS was providing a first-class neutron scattering facility.

The capabilities are excellent but aging. There are several instruments on Target Station 1 that are long overdue for an upgrade (IRIS, OSIRIS and SANDALS being the most urgent ones). Investment in new instrumentation on TS1 is urgently needed. ISIS's capabilities are now matched, and in some cases exceeded, by those at J-PARC and SNS. This process will be accelerated with the arrival of ESS. Investment in instrumentation is key to maintaining ISIS's world-best position.

The facilities are world-leading in terms of the instruments and experienced personnel that support each instrument and area. The opportunities for world-leading research to emerge from ISIS are limited primarily by the beamtime available. From my experience of sitting on selection panels, there are almost always more excellent proposals than there is time to do the science.

Generally, yes. There is a constant need to review performance as compared to other facilites and the demands of the science proposed. Flux, resolution and temporal performance in terms of data collection and processing are all key factors. As a materials chemist working at ISIS, sample environment is also crucial in stretching the limits of the science that can be performed. This is an area in which ISIS also excels and it needs to continue to have the time and funding to allow experimentalists to realise the ground breaking work that the might propose.

The capability of the instruments on ISIS Target Station 2 are outstanding. The instruments on ISIS Target Station 1 are also excellent, but the SNS (Oak Ridge) and JPARC (Japan) spallation sources are becoming more powerful. If there is an opportunity to upgrade Target Station 1 (and I understand that there is) then it would be very good value to do it.
ISIS: The capability of the instruments on ISIS Target Station 2 are outstanding. The instruments on ISIS Target Station 1 are also excellent, but the SNS (Oak Ridge) and JPARC (Japan) spallation sources are becoming more powerful. If there is an opportunity to upgrade Target Station 1 (and I understand that there is) then it would be very good value to do it.
ILL: world-leading for most instruments I use
Diamond: All instrument I use are comparable to the best in the world
ESRF: Instruments I use are the best in the world.

The facility is over-subscribed, so you will often get less days than you request in your proposal; yes, it has got low temperature, high magnetic fields and high pressure capability, plus a laser facility

Very useful, but the imaging facilities promised for next year will be even more useful for our purposes; Yes, but imaging will be very welcome, for Cultural Heritage objects.
The distribution of phases within historic steels as well the detecting of their presence should enable us to determine more about manufacturing techniques.

The instruments that I use are operating well and should remain world leading or internationally competitive on at least a 5 year time scale; I think the instruments are excellent, but there is not enough time available for all of the excellent science being undertaken.

Present capability of the Central Facilities is just enough to satisfy current user demand. However in nearest future the demand is going to rise (especially in neutron scattering area) and Central Facilities might experience some problems to satisfy the demand.

- *What developments in Central Facility capability would you like to see initiated over a 5-10 year time horizon?*

At ISIS, a biology lab (allowing eukaryotic cell culturing) would be useful

TS1 upgrade, participate in ILL and ESRF as long and strong as possible, ILL endurance program, and ESS!

In-operando and combined measurements. Remote access.

Perhaps greater availability of sample environments for high pressure, flow.

I am pleased with a number of developments that I happen to know are in the pipeline. It is important to have folks trying new approaches and ideas as it is essentially impossible to know what will be required in the future. I would also add that it is essential for us to have a steady accessible supply of beamtime, even if not at the highest flux or related superlatives. We need to maintain an active research group activity, particularly with our projects with industry, and one VERY high flux source will NOT be a benefit if we end up with less actual access. (In a similar fashion we do a lot of synchrotron experiments, generally the flux is not the main issue controlling the rate of an experiment).

The key to improving instrumentation is more detected flux. The most cost-effective way to do this is provision of neutron guides on (most) instruments. Increased detector coverage is also very effective. The proposed TS1 upgrade does not represent good value for money in terms of increased capability (although it may be needed for sustainability). Flux improvements need to be complemented with increased manpower; the bottleneck to production of output is data analysis/modelling.

The ability to collect data over order of magnitude lower timescales and to couple multiple techniques on single instruments. Hence, one could conceive of following the making and breaking of bonds across multiple length scales, for example, and probing the changes in physical properties as a result.

1. Upgrade of Target Station 1 at ISIS; 2. Build a medium energy RIXS instrument at Diamond

Better SAXS and SANS capability in the UK

Another low transverse field muon beamline, as the oversubscription for MuSR is always double the number of days.

I would like to see instruments with even better capability for evidencing very low magnetic moments (neutron scattering). I would like to see more physical property measurement equipment (PPMS/SQUID) at ISIS so that complementary studies can be made. It is excellent that such facilities are there at present, but it is very oversubscribed.

ISIS neutron source: Refurbishment of the older ISIS instrumentation is becoming an urgent need. Although most ISIS instruments are still providing state-of-the-art capabilities in neutron total scattering methods, they will not be able to remain at the forefront of the field beyond a 5 year timescale. Significant investment in technical optimizations of the instrument suite is required to maximize the scientific benefits that can be delivered from the facility's neutron target stations. This is particularly important if data quality is to be maintained at acceptable levels from the ever more challenging systems that are being investigated.
Diamond: To maintain a competitive edge, the physical sciences beamlines at Diamond need to be equipped with detectors of comparable quality to the world leading devices that the facility is purchasing for its life-science instruments. The physical science beamlines at Diamond often appear

to be equipped with cheaper and lower quality detectors, not just within Diamond but also when compared to many of the competing synchrotron facilities around the world. Examples would be (i) in X-ray spectroscopy Diamond has equipped its dilute spectroscopy beamline with a 64 element fluorescence detector, when competing facilities are purchasing 100 element detectors to allow them to push detection limits to lower levels, (ii) with the newly constructed total scattering beamline XPDF, the instrument is being equipped with cheap CCD based flat panel detectors, whilst it is standard practice on the life science instruments at the same facility to purchase single photon counting Pilatus devices for ten times the cost. Such decisions in physical sciences are not the route to world-beating capability. It seems a real shame for the facility to invest huge sums of money in world beating beamline optics, only to then sacrifice most of the gains through poor detection capability.
ESRF: Comments about the quality of the detectors offered to physical science beamlines at the ESRF would mirror my observations about the situation at Diamond.

- *Propose areas of activity that you believe will be important in terms of scientific advancement up to (i) 2020 and (ii) beyond.*

Development of anticancer drugs - defining pharmacokinetic and pharmacodynamic behaviour;
Studies of water behaviour (structure and dynamics) within human cells (e.g. cancer cells);
Osteometrics in human skeletal remains.

I) Quantum science. Energy; II) In-situ studies of devices.

In-operando and combined measurements. Remote access.

New materials for applications requiring unusual combinations of strength, density, conductivity etc.

(i) supercapacitors/biomaterials; (ii) biomaterials

1) CO2 separation, sequestration and utilisation; 2) novel battery materials

(i)/(ii) Bridging the gap between bulk, surface and cluster chemistry and resolving structure across nano length and timescales.
(i) superconductors, emergent phenomena due to electronic interactions in solids, topological materials, functional materials
(ii) All the above + quantum effects

Surface Analysis

Solid state chemistry of materials for energy and electronic applications

Understanding exciton interactions in different systems, including photochemistry, semiconductors, bacteria and photo-induced magnetism

Cultural Heritage: We are examining some of the 2000 objects in the Oriental Armoury of The Wallace Collection. This Non-invasive analysis is crucial in determining their constitution (and hence, possibly, their origin). Neutron diffraction has already provided us with a method of determining whether a "Damascus" pattern in present in a blade, but presently hidden from sight by Victorian mishandling. The anisotropic distribution of cementite seems to be related to the forging temperature, which in turn could provide a means of identifying workshops.

I am a solid state chemist with interest in magnetic materials for applications in magnetic memory, superconductivity and novel intermediate fuel cell electrolytes. Neutron diffraction is required to

determine crystal and magnetic structures of the new materials. I think energy materials such as Li ion battery materials, solid oxide fuel cell materials (anode/cathode/electrolyte), novel superconductors and water splitting materials will be important beyond 2020. Instruments with capability for pdf analysis will also be more and more important.

Areas of activity that I believe will be important: superconductivity, magnetism, bio-physics and soft matter, engineering science, chemistry & catalysis, clean energy.

- *Do you believe that STFC is fulfilling its role of providing Central facilities to a satisfactory degree? If not, what should it be doing differently?*

On the whole I believe that STFC is fulfilling its central facilities role at an appropriate level, but there are worrying signs that clear scientific vision and an ambition to be the world's best, is rapidly being lost from the senior management teams.
The general consensus was that STFC was doing a good job in managing the ISIS Facility.

Yes, although it appears that funding and staff numbers are very much a rate limiting factor for new developments. They could achieve more, with more!

Yes! I must say we are very pleased with the ISIS facility. This is something we can really be proud of on a world stage. Like all facilities such as these there are fluctuations of one aspect or another. However, I genuinely have the impression the staff and scientists at ISIS really want us to do well in our experiments and do their level best to help us do that. They are dynamic, capable and responsive (NOT all facilities we have used over the years are like that!!)

Generally yes. In my experience the facilites interact with and involve its user communities very effectively. This is certainly true of ISIS. My only serious concern is the economically-enforced restrictions on available beamitme as discussed above and the implications that the UK could be left behind from a position of historic strength...

One important thing STFC could do to improve the output of its Central Facilities:
Provide more studentships for graduate students in partnership with Universities, not necessarily tied to instrument development. Students working on pure science will become the next generation of researchers.

It is OK, but funding international facilities must be core to the stratergy

3.3 Laser Sources (2 respondents)

Two usable responses, both from IR spectroscopists. Both from Diamond users: one respondent in life sciences, the other a solid state chemist. The responses were complementary of the facilities and facility staff.

Do the LCF's provide state of the art capability?
Both responses were positive.
Both respondents replied that they would like to use live micro-organisms

Responses noted from other sections (of relevance to lasers)

- Some noted that there was a general lack of support staff (certainly true at CLF).
- It was noted that some of the facilities are over-subscribed and under-utilised (mostly in context of ISIS but also true of CLF)
- There was some desire for dedicated XUV/SXR beam lines, but no mention was made of Artemis which can cover some of this area.
- There was some mention that the IR beamlines are now competing directly with lasers (QCL) but that there main selling point can be synchronisation with other sources. Again Artemis might have applications in some of these areas.

3.4 Other (4 respondents)

4 responses from Universities of Oxford (2) and Southampton, and the Indian Institute of Science Education and Research Thiruvananthapuram. The respondents were all synchrotron users (or potential users) at Diamond or ESRF. The primary instruments used are:Beam lines Diamond 108, MX, cryoEM. Research areas covered are: (i) Environmental research (2); (ii) Development of electron optical instrumentation, (ii) imaging, theory, cryogenic optics; (iv)Genomic stability in humans. Overall the respondents were happy with the present and future capability of the facilities, rating them as "Excellent" or "World Class". Only one respondent suggested a development on the 5-10 yr timescale (shipping of Dewars).

Chair: Professor David Lennon – Glasgow University
Dr Howard Stone (Deputy Chair) - University of Cambridge
Mr Colin Danson - AWE (Aldermaston, Reading)
Prof Mike Fitzpatrick - University of Coventry
Prof Konstantin Kamenev - University of Edinburgh
Prof Sue Kilcoyne - University of Huddersfield
Prof Peter Lee - University of Manchester
Prof Zulfikar Najmudin - Imperial College London
Prof Paul McMillan - University College London
Prof Andrew Orr-Ewing - University of Bristol
Prof Paolo Radaelli - University of Oxford

D. Lennon (3rd February 2016)