STFC Physical Sciences and Engineering Advisory Panel
Report to the Large Facility Sub-Group

Overview

The Physical Sciences and Engineering Advisory Panel (PS&EAP) was tasked with providing an overview of scientific priorities for a number of large-scale Central Facilities (CFs) within the STFC portfolio (Diamond, ISIS, CLF, ESRF, ILL). Guidance was sought from a short term perspective (0-5 years) and a longer term perspective (5-30 years). The work for the Advisory Panel (AP) could be partitioned within the following three categories:

- Photon sources for Physical Science and Engineering
- Neutrons and Muons for Physical Science and Engineering
- Laser sources for Physical Science and Engineering

However, in order to better assist with defining STFC's connectivity with the other Research Councils, the various work programmes were sub-divided into the six headings of the RCUK Excellence and Impact agenda, as outlined below:

- Digital economy
- Energy
- Global food security
- Global uncertainties; security for all in a changing world
- Living with environmental change
- Life long health and well being

Following guidance from the STFC Secretariat and in agreement with the Life Sciences and Soft Matter Advisory Panel, a table format was adopted which was intended to address items (a)-(d) as indicated in 'Guidance Notes For STFC Advisory Panels Related To The Facilities For The Programmatic Review' [LFAP(12)2 (October 2012)]. At a meeting of the PS&EAP in October 2012, the STFC Secretariat agreed that the AP was not required to produce a rank list of priorities. Nevertheless, the examples presented herein are thought to reflect the highest priority topics that are linked to STFC's portfolio of interests in Physical Sciences and Engineering.

Although the majority of topics reviewed could be accommodated within the tabulated format, certain topics required extra justification. This material is therefore presented within a series of seven appendices that follow on from the tabulated information. These appendices are listed below.

1. The ESRF as a resource for the UK scientific community
2. A medium-term perspective on the provision of neutrons at the ISIS Facility
3. The ESS as a resource for the UK neutron community
4 Laser driven science;
    (a) Overview
    (b) Combining lasers with synchrotron or neutron beamlines
    (c) Free Electron Lasers (FELs)
    (d) Medical applications of high power lasers.
5. Heritage science.
6. Research Council interfaces
7. Universities as direct stake-holders in Central Facilities

The skills-base inherent to the AP was insufficient to cover all of the subject areas within a Physical Sciences and Engineering remit. Consequently, the AP has consulted with a number of UK academics on specific topics, with those inputs inserted into the documentation without accreditation. The contributions from those valued colleagues are greatly appreciated.

Finally, it is noted that the APs are expected to be active at least on the medium-term. It is acknowledged that a task of the APs is to "consult and interact with the community to ensure that its views are canvassed" [LFAP(12)2 (October 2012)]. Whilst it was not possible to consult with the whole CF user community within the life of the AP (initial activity August 2012), it is expected that this AP guidance document will eventually be publicly disseminated. At that stage, it will then be appropriate to run a planned consultation exercise; the feedback of which will inform the AP guidance for the next round of consultation in to Science Board (2013/14). In this manner, it is hoped that the APs will be deemed to be credible by their peer group and also transparent in their operational procedures.

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Tuesday 15th January 2013

1 Digital economy

No.	Scientific and / or technological challenge	Timescale Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	Research Council priority area?	Facility(ies) currently used	Facility(ies) required for future research including any new technological development / upgrades)	UK position (e.g. world leading, internationally leading, nationally leading etc.)	Potential economic impact including expected timescale to deliver	Potential industrial impact including expected timescale to deliver
1.1	Novel electronic/magnetic phenomena; quantum phase transitions; information storage/quantum computing. [Community size: medium]	Mid-term	Mainly EPSRC but also EU and other international sources	ISIS, Diamond, ILL, ESRF	Especially if ISIS TS2 fully implemented, and Diamond Phase III beamlines completed, along with maintaining/ strengthening UK participation in (upgraded) ILL/ESRF most facilities in place.	UK activity world leading especially at neutron/muon and synchrotron sources. Fundamental physics/nanoscience with potential technology impacts. Possible Nobel-quality research ?	Industry interest via nanotechnology centres: research still mainly academic but potential technology development on 15-20 yr horizon	Applications down stream of thorough academic work could be significant would require substantial industrial development. Noteable outcomes anticipated within 10-20 year timescale.
1.2	***Complexity and emergence*** This field of research lies at the fundamental end of the spectrum. Strong interactions between electrons and ordinary excitations can result in *exotic ground states and excitations*, behaving according to models often developed for elementary particles physics. [Community size: small]	Long term	EPSRC Physics Grand Challenge: **Emergence and Physics Far From Equilibrium**	All large-scale facilities	All of the above plus FEL & X-FEL	World leading in many areas. Good scientific expertise in FEL/X-FEL but need acces to source to develop community	Long term, mainly in industries that do not yet exists.	Credible industrial impact in the field of quantum computation and QIP in general. This could be delivered in the next 5-10 years.
1.3	***Novel materials and Functional materials***. Materials such as high-temperature superconductors, have the potent to generate transformative technology. There is often no consensus on a	0-5 years all the way to long term.	EPSRC Physics Grand Challenge: **Quantum Physics for New Quantum Technologies**	All large-scale facilities	All of the above plus FEL & X-FEL	World leading in many areas. Good scientific expertise in FEL/X-FEL but need access to source to develop community	Medical imaging, low-temperature devices, information storage and processing.	Hard to predict, as novel materials are typically in pre-competitive research. Could happen very quickly if a market beater is found.

	comprehensive theory describing these phenomena, so these subfields are experimentally driven. Although the physics of ***functional materials*** is well established, unexpected manifestations of their properties lead to novel phenomenology, which can inspire new device concepts. [Community size: medium]							
1.4	***Device physics*** is the study of functional materials patterned in a device-like assembly with feature sizes of the order of tens of nanometres. [Community size: medium]	0-5 years all the way to long term.	EPSRC Physics Grand Challenge: **Quantum Physics for New Quantum Technologies**	Synchrotron radiation. Fundamental materials development done also with neutrons	FEL/X-FEL will be important	Not as strong as the other fields, due to the weakness of industrial base	Information storage/processing. Medical diagnostic.	For example, Toshiba is developing new smart memories and transistors based on magneto-electric switching of TMR junctions.
1.5	Novel functional material development, Quantum Physics for New Quantum Technologies, Emergence and systems far from equilibrium via application of muon spectroscopy [Community size: small] N.B. Section 1.5 differs from 1.1-1.3 as it exclusively uses muon spectroscopy.	5-15 years	Yes, EPSRC and STFC	ISIS- Muon spectroscopy	Continued access to beamtime (more operational days) plus continued investment in sample environment.	The UK has the world leading pulsed muon source at ISIS and this capability favours experiments which either utilise the pulsed structure of the beam or those that take advantage of exceptionally high data rates provided by pulsed sources compared to continuous ones.	This capability has helped the UK take the lead in exploration of new superconductors and magnets by efficient mapping of phase diagrams and probing of new magnetic ground states. Taken hand-in-hand with a renewed focus on materials development, this promises to be a substantial growth	The development of pump-probe (electric field, laser, microwave pulses) technologies that have the potential to open up new areas of science, both underpinning and exploratory. The science areas which are impacted by these developments include: molecular science, spintronics, frustrated magnetism, superconductivity, multiferroics,

							area and one in which high-impact science will be generated.	functional materials, chemical kinetics, soft matter. Companies such as Oxford Instruments are well placed to exploit these advances.

2. Energy

No.	Scientific and / or technological challenge	**Timescale** Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	**Research Council priority area?** (Yes/No; state which RC)	Facility(ies) currently used	Facility(ies) required for future research including any new technological development / upgrades)	UK position (e.g. world leading, internationally leading, nationally leading etc.)	Potential economic impact including expected timescale to deliver	Potential industrial impact including expected timescale to deliver
2.1	Properties of warm dense matter – Of central importance in fusion science, laser-plasma science, laboratory astrophysics. [Community size: small]	Near/ mid-term	**Energy** *EPSRC Physics Grand Challenge: Emergence and Physics far from Equilibrium*	Vulcan Astra-Gemini Flash LCLS	Vulcan 10PW LCLS/LCLS II XFEL UK NLS	World leading (but position will weaken if we cannot ensure access to XFEL's)	Underpinning to inertial confinement fusion (long term) Stock-pile stewardship Near and mid-term	Long term impact on industrial development of fusion power
2.2	New technologies for accelerators based on laser-plasma interaction – Of importance to new imaging technologies, compact accelerator technology, healthcare technologies. [Community size: small]	Mid- / Long term	**Lifelong Health….** *Health Care Technologies (EPSRC)*	Vulcan Astra-Gemini	DIPOLE Vulcan 10PW ELI Hiper	Internationally leading (but will lose this position without suitable investment in world class laser facilities)	Proton beams for[1] therapy (10-20 years) Electron beams for new light sources[2] (20-30 years)	Compact accelerators for portable proton, ion and X-rays may revolutionise in-situ diagnostics e.g. in oil industry Long term
2.3	Development of (laser-driven) Inertial Fusion Energy. This requires high power high rep rate lasers in the Megajoule class as well as mass production of targets designed for high gain. Outcome is clean zero carbon fuel source. [Community size: small]	Long Term for fruition. Beneficial economic impacts would be felt in near and mid term too	**Energy**	(Vulcan and Omega in the US have been used to stage for) NIF which is designed to demonstrate fusion gain. CLF Dipole system is demonstrating the possibilities	Once NIF ignites, the next step will be to build a working reactor (HiPER/LIFE projects). Further (Dipole-like) laser developments required in pumping to get high power high rep rate. Target design and mass production facility will also be required	UK is internationally leading, in part due to HiPER but also as a P5 nation with HEDP/Laser expertise	If the UK leads in this area, perhaps leading a European programme, then this will lead to huge economic impact due to jobs and IP	Industrial impact is huge for the same reasons. Investment in laser technology, mass target manufacture and reactor design would secure a stake in IP licensing of power plants, giving UK "supplier" rather than "customer" status.

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[1] There are still technology problems to be solved such as reliable high rep-rate, high power lasers, and scientific issues regarding achieving the necessary acceleration, energy bandwidth and beam emittance. This puts this work firmly in the research rather than the facility development category.

[2] The electron beams so far generated are neither sufficiently energetic, monochromatic, low emittance or stable to drive a FEL, but with more research and development we may be in the position to plan a facility based on this technology in the longer term.

				of diode pumped lasers				
2.4	High rep rate high power laser technology [Community size: small]	100J:2 years Shortpulse: 3years 1kJ: 5 years	**Technology development by STFC for exploitation by other councils later.**	Vulcan and Astra Gemini already deliver high peak power where shot rates are limited to hours and minutes.	Combination of high peak power with high average power to enhance process throughput. DiPOLE strategy is aligned to this.	World leading	DiPOLE has won competitive contracts in excess of £2M and is currently negotiating a £10M contract with ELI Prague.	The high rep /low peak power market and the low rep / high peak power markets are worth billions p.a. High rep high peak power would merge the existing markets and create new ones.
2.5	Ultra-high intensity laser / matter interactions [Community size: small]	The case has been thoroughly reviewed and given the highest priority – very achievable in the near term.	**Technology development by STFC for exploitation by other councils later.**	Vulcan demonstrated PW performance	Vulcan 10PW has been fully planned for some time, and will probably be sufficient to allow 20PW to be attained.	In a strategic context, delivery of the 10PW upgrade to VULCAN is required to maintain the UK's undisputed world leading position. Note that the ELI facility plans will not deliver the user environment (ops, training) for UK users	Sample impacts in the examples below	Sample impacts in the examples below
2.6	Fusion by direct laser acceleration. DT nuclei, oscillating in a laser beam can encounter each other with sufficient energy for fusion [Community size: small]	Near term	**Energy**	Vulcan can achieve 10^{20}W/cm^2 too low for significant fusion.	Vulcan 10PW could provide10^{22}W/cm^2 which would put DT ion energies at a peak in the cross section, allowing study of a novel thermonuclear mechanism. Also for fusion of other low Z nuclei.	This would be a novel application	Science impact first	Possible IFE/MFE applications in improved understanding.
2.7	Ultrafast electron dynamics [3] [Community size: small]	Near/Mid Attosecond dynamics of electrons in molecules Correlated electron dynamics	**Energy** **Lifelong Health…** *Health Care Technologies*	Artemis Astra-Gemini	Attosecond sources High harmonic generation sources 2D UV and 2D UV/vis spectroscopy[4]	Internationally leading – field is beginning to open up and UK science is currently well	Economic benefits include improved solar energy capture (e.g. exploiting	Energy sector 5-15 years

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[3] The required temporal resolution is <10fs, this connects to the Dynamics of Photodriven Processes where even faster timescales are needed and where the structural information is not always of critical importance.

		Orbital tomography Light harvesting / solar energy capture	*(EPSRC)* *EPSRC Physics Grand Challenge: Emergence and Physics far from Equilibrium*			positioned but will rapidly lose competitiveness if access to XFEL is not ensured	coherence in the electron dynamics) 5-15 years	
2.8	New materials discovery and development for energy science and sustainability: includes catalysis, photocatalysis, battery/fuel cell research, biomass conversion, greenhouse gas reduction. Basic and applied research combining chemistry, physics, materials science/engineering: many fundamental challenges and scientific breakthroughs to be made involving academic + industry partners. Major UK, EU and international public policy/society drivers [Community size: large]	Much current activity in UK and internationally: rapid growth expected over next 5 years and UK should take advantage of current leading positions in areas including battery materials, H2 storage/production; biomass conversion; energy-efficient catalysis: expected coninued development throughout 5-15 and 15-30 yr horizons as new research directions/technology developments/industry outcome come into play	Major RCUK themes (e.g. energy) : mainly supported by EPSRC and also EU	Diamond, ISIS, ESRF + also APS, Spring-8); ILL; uses Harwell Research Complex (HRC): X-ray and neutron beamlines used for in situ materials characterisation during synthesis, processing and materials function: diffraction, imaging and spectroscopy. Increasingly match beamline capabilities with on-line experimental studies and nearby research centres (e.g. HRC; ESRF Science/Technology buildings)	Must make sure that existing (phase I/II as well as approved phase III) Diamond beamlines are fully operational and supported; continue to implement ISIS TS-2 (detailed beamline plans are in place). Must take full advantage of ESRF upgrade for nanoscience/ imaging, in situ/extreme conditions research; advanced spectroscopy capabilities (should re-negotiate increased UK contribution ? also discuss spread of UK beamline access ?).	Internationally/world leading in several science areas (battery/ fuel cell research; catalysis/photocatalysis etc): also in technology development, SME and start-up activity as well as large companies	Very high value strategic sectors for UK economy; internationally legislated targets for achieving materials performance: some industry uptake already based on basic science results combining lab and facility research; considerable industry interest, and expected real outcomes on 5-10 year horizon.	see column to left

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[4] Although 2D IR spectroscopy is becoming an established method at ULTRA, 2D UV is not yet active within the UK but offers new insights into coherent electron/molecule dynamics.

2.9	Gen IV/fusion reactor materials [Community size: small]	20+ years	EPSRC and STFC (energy)	ISIS, Diamond, ILL, ESRF	More flux, more resolution. Also, neutron irradiation facilities and hot cells on Harwell site using spare ISIS neutrons in target area?	Internationally competitive	Industrial-scale power for a low carbon society, with intrinsically safe, low waste reactors (can survive loss of coolant)	Gen IV reactors are ~20 years Fusion: ITER, DEMO through to deployment is 50 years.
2.10	Safety evaluation of welds in UK power plants [Community size: small]	0-30 years	No	ISIS (Engin-X)	Precision sample manipulation equipment capable of performing operando measurements (e.g. temperature and/or pressure).	World leading	Companies such as British Energy currently use ISIS to evaluate safety cases for welds in corrosive environments. This information directly connects to the safe operation of the UK electrical generation network.	Improved capability in this area would lead to improved sustainability of the UK electrical generation base, with downstream benefits to the whole UK economy. This important work is often not well recognised as it is undertaken outside the User programme.
2.11	Analysis of 'functional materials' via Inelastic neutron scattering [Community size: small/medium]	5 - 30 years	STFC – Y EPSRC – Y (Condensed matter component of Physical Sciences programme)	ISIS	ISIS is currently world-leading but other facilities are catching up and a small number of units overseas (e.g. SNS, ESS, J-PARC) could overtake ISIS's role as the premier place to undertake a range of neutron scattering experiments. How many areas of scientific endeavour is the UK genuinely world-leading? Not many. Investment now, planned for a 20 year time horizon, is required to up-grade the ISIS Facility, see Appendix 2.	Unless the up-grade in neutron flux by up-grading TS-1 is undertaken then ISIS will become increasingly ineffective as a site for cutting-edge INS measurements. Something else that would assist INS in maintaining a competitive edge for global neutron scattering studies would be to invest in further Sample Environment capacity. This	Such an investment now would send out the statement that ISIS seeks to remain world-leading. That would bring the world's best neutron science to Didcot! This science would be diverse and high quality with expected benefits likely to accrue in 5-10 year time period.	Significant advances anticipated in hydrogen storage options, fuel cell technologies, chemical processing options (e.g. catalysis), biological applications, etc. An example of an area that has great potential to deliver tangible benefits to mankind and the economy is the investigations of high Tc superconductors. Fundamental studies in this area are improving the understanding of issues constraining elevated Tc's. A

						would enable more elaborate experiments to be taken to the neutron spectrometers. A modest investment in that area of user support could deliver significant scientific output not readily attainable under current arrangements.		breakthrough, such as accessible superconducting devices capable of operating at liquid nitrogen temperatures, would mitigate against the current reliance on helium which, as recent events have shown, is a restricted resource. The UK needs to maintain its world-leading position in this highly important research area. Magnetic measurements via neutrons are an important part of that skills-set.
2.12	Intermediate temperature proton conductors [Community size: small]	5-20	STFC and EPSRC – not explicitly stated but topic falls within Energy agenda of both RCs.	ISIS Little research in UK on this particular topic. Major research effort within Japan and parts of Europe (e.g. Switzerland). This is an area ripe for exploitation via neutron scattering.	ISIS, elastic and inelastic neutron scattering spectrometers. This represents an opportunity for the UK to open up a new area in power devices, something vital for the forthcoming changes anticipated within the energy landscape. Intermediate temperature (200-400°C) proton conductors are comprised of heavy metal oxides (e.g. Ba $In_xZr_{1-x}O_{3-x/2}$) plus water with hydroxyl groups acting as charge carriers. These materials are components in candidate intermediate temperature fuel cells, which avoid many of the	No strong UK activity at present. Solid oxide fuel cells are well studied (UK and elsewhere) but require high operating temperatures. The proposed area of *intermediate temperature proton conductors* provides an opportunity for the UK to contribute to a research area	Given the limited range of information currently available on this important topic, it is expected that high impact academic publications would flow from the earliest stages of any investment in this area.	Within a 5 year period, one envisages patents being filed for high performing electrolytic membranes, providing a platform for industrialists to engage in future research programmes. Unless this happens, it is most likely that future UK users of fuel cells operating in this temperature regime will be using technology licensed from Japanese manufacturers.

					problems connected with the more conventional (high temperature) solid oxide fuel cell.	with real industrial application.		

3. Global food security

No.	Scientific and / or technological challenge	Timescale Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	Research Council priority area? (Yes/No; state which RC)	Facility(ies) currently used	Facility(ies) required for future research including any new technological development / upgrades)	UK position (e.g. world leading, internationally leading, nationally leading etc.)	Potential economic impact including expected timescale to deliver	Potential industrial impact including expected timescale to deliver
3.1	Optimisation of catalysis linked to integral parts of process chains for argi-chemical production. [community size: small]	Current activities centred around the application of heterogeneous catalysis in a few key processes, e.g. selective hydrogenation. However, mid-term work will concentrate on (i) process intensification strategies and (ii) catalyst deactivation.	EPSRC and BBSRC	ISIS	More sensitive neutron spectrometers at ISIS.	A small number of UK academic researchers are well connected with industry, however, consulting companies such as Solvias (Switzerland) tend to dominate interactions with the large argri-chemical manufacturing companies in this area of applied science.	UK researchers are already solving industrial problems and improving atom efficiencies of large scale production of plant-protection products. Economic benefits (to industry) are significant. The resulting new technology is also potentially licensable, providing greater economic impact.	Access for UK users to more sensitive instrumentation (e.g. similar to specification of SNS SEQUOIA spectrometer) would enable more catalytic systems to be investigated. Timescale dependent on ISIS up-grades.

4. Global uncertainties; security for all in a changing world

No.	Scientific and / or technological challenge	Timescale Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	Research Council priority area? (Yes/No; state which RC)	Facility(ies) currently used	Facility(ies) required for future research including any new technological development / upgrades)	UK position (e.g. world leading, internationally leading, nationally leading etc.)	Potential economic impact including expected timescale to deliver	Potential industrial impact including expected timescale to deliver
4.1	X-ray imaging at high rates could be developed by targeting a high power high rep rate laser onto appropriate targets. [Community size: small]	Near term	**Technology development by STFC for exploitation by other councils later.**	High rep rate laser systems, e.g. DiPOLE.	High rep prototype is Dipole system.	Dipole is in the forefront of diode pumping required for high rep rate systems	Not only the system, but the improvement in technologies on which it provides subsequent info. Imaging for defence technology.	Imaging internals of machines in use would have widespread application
4.2	National Security. Lasers allow access to high energy density physics enabling the safety and security of the nuclear deterrent to be maintained in the Comprehensive Test Ban treaty era. Provides material data as well as computer code validation in a pertinent regime [Community size: small]	Near term	**Global security**	Orion laser has just been commissioned for this purpose at AWE, also NIF in the US	No further UK development required until Orion life is extended in 2020.	World leading as a P5 nation, and a unique facility in Orion, though not on the scale of LMJ or NIF.	90% of the money spent on Orion entered the UK economy	UK may be able to deliver consultation based on knowledge of laser design and delivery
4.3	X-ray tomography Imaging large-scale engineering structures: metal/ceramic fatigue; microstructures/textures in rock/ceramic samples; 2-D and 3-D tomographic imaging of synthesis/ catalytic reactors under industry/operando conditions [Community size: large]	UK is pioneer/ international leader in this area, ranging from studying fracture/failure mechanisms in large scale engineering structures (aeroplane wings, turbines, reactors etc); uses neutron (ISIS, ILL) and high-energy X-ray (ESRF, Diamond) sources to penetrate/map large samples including real large-scale: detector	Yes. STFC and EPSRC	Diamond, ILL, ISIS.	Activities at ILL, ISIS and Diamond require continuous support. The secondment of industrialists to Central Facilities could lead to greater integration between industry and academia. Correlative imaging where electrons and x-rays or neutrons and lasers say are brought to bear on the same sample to provide complementary insights. This concept is now realisable at the	World leading. It can be used to study degradation for example of osteoporosis, or the subsurface degradation of aeroengine turbine blades or materials for nuclear application under intense radiation doses. It can help	This area of engineering has direct impact on a wide range of areas. The level of current industrial support (e.g. Rolls-Royce, Airbus Industries, etc.) is evidence enough of its relevance to engineering led commercial organisations.	see column to left

		development for rapid 2-D/3-D tomography. In situ studies during pharmaceutical processing, nanoparticle synthesis, catalytic reactors etc. Massively important materials/ mechanical/chemical engineering area supported by industry: also environment/ planetary science applications.			Harwell Complex.	us to understand how damage accumulates and when to judge when to remove a material before it comes unsafe or to develop strategies to stall degradative processes whether they be in medicine or engineering.		

5. Living with environmental change

No.	**Scientific and / or technological challenge**	**Timescale** Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	**Research Council priority area?** (Yes/No; state which RC)	**Facility(ies) currently used**	**Facility(ies) required for future research including any new technological development / upgrades)**	**UK position (e.g. world leading, internationally leading, nationally leading etc.)**	**Potential economic impact including expected timescale to deliver**	**Potential industrial impact including expected timescale to deliver**
5.1	Ultrahigh (GigaGauss) magnetic fields. A magnetic field of this strength cannot otherwise be generated in the lab. [Community size: small]	Near term	**Basic Science**	Vulcan short-pulse experiments at 10^{20}W/cm^2 have delivered hundreds of MGauss.	Vulcan 10PW would provide10^{22}W/cm^2 which would deliver GigaGauss fields, pertinent for white dwarf and neutron stars	Currently theory of white dwarf and neutron star fields not experimentally underpinned.	GigaGauss fields would be world leading	Access nto highest magnetic fields may be relevant to future technologies in many sectors.
5.2.	Laboratory Astrophysics and planetary physics. Accessing temperatures of 5 to 10 million degrees in material at solid density is pertinent to the cores of large planets and stars leading to improved stellar astrophysics models. The ability to generate magnetised plasma jets provides a scaled model for nebulae, for example. [Community size: small]	Near term	**Basic science**	Vulcan, Orion, Omega in Rochester USA. Also FELs	Requires systems with combined short and long pulse beams for compression and heating , then diagnosis. Orion will serve the near term, but cannot meet the capacity for academic requirements with the 15% available programme time	Orion puts the UK in the forefront of world capability in these areas	Hot and Warm Dense Matter are poorly modelled being between regimes with tractable approximations in the physics	No direct industrial impact but improved understanding of physical phenomenon, which could have long-term environmental consequences.

6. Life long health and well being

No.	**Scientific and / or technological challenge**	**Timescale** Near term (0-5 years) Mid-term (5-15 years) Long term (15-30 years)	**Research Council priority area?** (Yes/No; state which RC)	**Facility(ies) currently used**	**Facility(ies) required for future research including any new technological development / upgrades)**	**UK position (e.g. world leading, internationally leading, nationally leading etc.)**	**Potential economic impact including expected timescale to deliver**	**Potential industrial impact including expected timescale to deliver**
6.1	Imaging cell function at the nanoscale with short wavelength light and high time resolution (soft X-rays/hard X-rays; 2-photon microscopy; high spatial res fluorescence imaging) [Community size: medium]	Near/Mid Correlated structural and dynamical information in bio systems Photodynamic therapy	**Digital Economy** **Lifelong Health…** **Energy** *Imaging for Biological and Biomedical Sciences*	Diamond/ESRF Astra/Artemis Flash LCLS SACLA LSF (ULTRA and Octopus)	Diamond/ESRF XFEL Swiss FEL SACLA UK NLS Combined CLF/Diamond	UK has an internationally leading biomedical imaging community. Need access to the best new technologies to remain competitive	Economic benefit in nanotechnology, biotechnology and medical areas	Biomedical sector 5-10 years
6.21	Fast dynamics/structure studies in biomolecular/ biological systems; studies of biomolecular structure/function [Community size: large]	UK internationally leading in several areas of biochemistry, biophysics, biomedicine; also pioneering in certain areas of biology e.g under extreme conditions relative to deep biosphere and origins of life. UK biomed research is world leading: Nobel quality.	MRC, BBSRC, EPSRC Also Leverhulme, Wellcome etc Also international sources (Sloan Foundation)	ESRF, ILL, ISIS, CLF (ULTRA and Octopus), Diamond just starting; FRM-II NLS should be developed as a major new tool enabling world class developments Provide core support for deuteration lab at ILL/Grenoble affiliated with ILL - this is world leading support facility supported via UK RC funds	See case made in NLS project document: also ILL/ESRF upgrade plans ; ISIS TS-2 and Diamond phases I-III	The interactions between Diamond and the CLF will lead to world-class science.	This are of research is already delivering now. Structural biology is at the centre of bio-physical research which is leading to new treatment protocols for particular diseases, new drug developments, new plant protection regimes (agri-chemicals) and an improved awareness of the mechanisms of life.	Medium term the benefits of this class of research are enormous. Drug development alone is a multi-million pound business that requires continuous research to maintain competitive advantage. The UK is a major world player in this area. Likewise agri-chemical research, development and production.
6.3	Medical treatments using ionising radiation	Near to mid term for development to uptake	**Lifelong Health**	Accelerators (laser	High rep rate high power lasers would provide compact highly	Dipole is in the forefront of diode	Improved medical outcomes would be	Construction of the systems

	[Community size: medium]			developments on Diploe system)	directable sources	pumping required for high rep rate systems	valuable worldwide	
6.4	Structural dynamics on timescales from fs to s [5] Following structural changes from the atomic scale to the meso scale in isolated molecules and condensed phases; "making molecular movies" Structural changes in solids and nanomaterials [Community size: large]	Near Gas and liquid phase chemistry Mid- Biochemistry and nanomaterials Light-harvesting / solar energy capture Photodynamic therapy Long- Following complex structural changes in biomolecules	**Energy…** **Lifelong Health….** *Health Care Technologies (EPSRC)* *EPSRC Physics Grand Challenge: Emergence and Physics far from Equilibrium*	ULTRA OCTOPUS Artemis Flash LCLS	Time resolved beamlines at synchrotrons Next generation ULTRA (THz to UV) Combining lasers and beamlines XFEL LCLSII NGLS (Berkeley) UK NLS Attosecond sources OCTOPUS invaluable for characterising samples and for sample manipulation	Internationally leading – field is beginning to open up and UK science is currently well positioned (e.g. in ultrafast IR spectroscopy and atto-seconds), but will rapidly lose competitiveness if access to XFEL is not ensured.	Economic benefits include in catalysis industry, understanding drug delivery and activity, control of properties of materials (e.g. superconductors) 5-15 years	Chemical, Biomedical, Pharmaceutical, materials technology sectors 5-15 years
6.5	Single molecule imaging with short X-ray pulses– Determining structure of non-crystallizable macromolecules e.g. membrane proteins [Community size: medium]	Mid/Long term	**Lifelong Health..** *Imaging for Biological and Biomedical Sciences* *Health Care Technologies (EPSRC)*	LCLS for preliminary studies	XFEL LCLS II SACLA Swiss FEL	UK is a world leader in protein structure determination. To maintain this we must stay abreast of new technology.	Economic benefits include drug development and biomedical area. 5-15 years	Pharmaceutical sector 5-15 years
6.6	Understanding Fatigue in titanium alloys → Utilising the full strength potential of titanium alloys in rotating parts in jet engines; providing higher fuel efficiency, lower air transport CO2 emissions; strengthening the UK aerospace sector. → deformation	5-20 years	EPSRC manufacturing the future Energy	ISIS, Diamond, ILL, ESRF	More flux, more resolution	World leading	Fuel savings, meeting UK CO2 commitments, UK jobs and supply chain. Knowledge economy etc. Need to keep up with 6.5% annual traffic growth globally.	Air transport is 7.5% of global GDP. RR, BAE and Airbus are the largest UK exporters, in a robust global innovation marketplace (GE, Boeing). Success in the next 5yrs, new alloys in 15, new products in

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[5] We envision using ultrafast pulses of X-rays or electrons for scattering and spectroscopy measurements. The use of FELs is critical to this mission, but other sources such as ultrafast high power lasers to generate X-ray/electron pulses are also important to this mission.

	mechanisms → tomography → diffraction contrast, coherence etc tomography → ordering, phonons [Community size: medium]							20. But incremental benefits in 5, 10 year timeframes.
6.7	Developing new, ductile, low density, creep and oxidation resistant high temperature materials (gas turbines) → diffraction → SANS/SAXS [Community size: medium]	15-20 years	EPSRC Energy	ISIS, Diamond, ILL, ESRF	More flux, more resolution	Internationally leading	As above	As above. 5-10 years to develop alloys, 5-10 to deploy in new engines and optimise.
6.8	Zirconium in the nuclear industry (and RPV steels) → Diffraction → SANS/SAXS → tomography [Community size: small]	5-30 years	EPSRC Energy	ISIS, Diamond, ILL, ESRF	More flux, more resolution.	Internationally competitive	Industrial-scale power for a low carbon society. Understanding evolution of materials in service and providing safety assurance.	Mobilising the UK nuclear manufacturing base – 5-10 years. Providing the assurance to pursue a nuclear power programme – all the civil and infrastructure investment in the UK that displaces fossil fuel imports.
6.9	Titanium and steels in offshore oil and gas. → Diffraction → SANS/SAXS → tomography [Community size: small]	5-10years	EPSRC	ISIS, Diamond, ILL, ESRF	More flux, more resolution.	Internationally competitive	Improving the profitability of UK domiciled oil majors (Shell, BP), increasing their UK engineering spend; high quality jobs and supply chain	Improving the profitability of UK domiciled oil majors (Shell, BP), increasing their UK engineering spend; high quality jobs and supply chain
6.10	Aerospace materials including new airframe with bonded crack retarders	5-10 years	EPSRC	ISIS, ILL	Additional flux for greater penetration	Internationally leading	Reduced weight of airframe leading to greater fuel efficiency and	Potential to revolutionise airframe designs by moving from riveted

	[Community size: medium]						reduced CO_2 and NO_x emissions	to welded constructions with lightweighting and cost reduction
6.11	Healthcare including biomaterials and implants [Community size: small/medium]	5-10 years	EPSRC BBSRC	ISIS, Diamond, ILL, ESRF		Internationally competitive	Ageing population requires implants and prostheses that will be developed from improved understanding of science	Changes to engineering new tissue to replace damaged or diseased bone will enable development of implants with greater reliability than existing technologies
6.12	Heritage Science [Community size: small]	Near to Long Term	No	Diamond and ISIS		Lagging internationally	No direct economic potential	Probably none
6.13	Developing structure-function relationships in new 'functional materials' – neutron diffraction [Community size: large] N.b. This activity is distinct from 2.11.	5 years	Yes, STFC. Strong connections to EPSRC.	ISIS, ILL	The ISIS instrument suite is well developed and nicely complements laboratory based X-ray facilities and syncrotron facilities (Diamond and ESRF). The community utilising these facilities is large and covers a broad area of science. Given the large number of scientists seeking to use neutron diffraction as a primary characterisation tool, an increase in the number of operational days at ISIS would lead to a significant increase in world-class science. Furthermore, an investment in sample environment would also be beneficial, permitting more elaborate *in situ* studies to be undertaken.	World leading	An extended number of operational days at ISIS would produce more high quality research publications detailing structural aspects of a variety of molecular systems. Some of these materials will have application in a wide range of commercial endeavours such as batteries, healthcare products, hydrogen storage devices, pharmaceuticals, etc.	Some materials under investigation are close to market and a heightened structural awareness could be exploited relatively quickly, i.e. within 5 years. An example is characterisation of a particular polymorph of a pharmaceutically active compound exhibiting favourable pharmo-kinetics. Due to associated engineering challenges, hydrogen storage devices such as metal hydrides, may take longer to bring to market.

Appendix 1
The ESRF as a resource for the UK scientific community

The European Synchrotron Radiation Facility was opened in 1994 as a shared research facility and is today supported by 19 partner countries (18 EU countries and Israel). It was constructed as the very first "third generation" (3-G) synchrotron using advanced insertion devices to generate intense and highly collimated beams of light extending from the X-ray to IR regions of the spectrum to carry out world-leading experiments in materials physics, engineering, chemistry and planetary sciences to soft matter and biomedical research. The pioneering research carried out by interdisciplinary teams from the member states and around the world has resulted in a large number of high profile publications featured on the covers of *Nature*, *Science* etc, patented technology developments and engineering solutions, and has contributed to the award of three Nobel prizes. The ESRF is located in Grenoble (France) as part of the EU "Science Polygon", alongside the Institute Laue Langevin's (ILL) nuclear reactor for neutron scattering, the European Molecular Biology Lab (EMBL) and other international facilities developed as collaborations among member states.

With an annual budget ~€80M the ESRF employs >600 people including internationally acclaimed scientists and engineers from throughout the EU. It supports the research of ~6500 user visits per year from about 4500 distinct individuals, who gain access to its unique experimental capabilities *via* competitively reviewed user access. Twice a year panels of international experts make recommendations for beamtime allocation to projects and these are then distributed across the available stations according to national contributions to the operating budget by ESRF management guided by its Council recommendations.

The initial ESRF project was based on an 6 GeV storage ring of 844m circumference leading to one of the brightest synchrotron sources available worldwide. The insertion devices that lead to the intense collimated beams of X-ray and other radiations were designed mainly around undulator systems leading to near laser-like beam qualities that can be directed at samples for diffraction, imaging and spectroscopy experiments with spatial resolutions extending down to the nanoscale. Many novel experiments have been designed around the unique beam characteristics, and the capacity for penetrating sample environments for *in situ* studies. These capabilities have only now been achieved at a few other synchrotron sources worldwide, including the Advanced Photon Source (APS) at Argonne National Laboratory (USA), Spring-8 (Japan) and now Petra-3 (Germany). The extremely high brilliance, focusing capabilities and the opportunity to devise and develop new classes of synchrotron experiments at the ESRF has led to pioneering and world-leading research and technology development by collaborative teams from throughout the member states. The UK has been one of the main beneficiaries of the ESRF project based on its large member contribution (14% until 2011) that was only matched by France, Germany, and Italy, and leading UK science teams from academic institutions and industry have developed world class research in fields ranging from quantum computing to materials for energy and biotechnology.

By early 2002 ESRF along with scientific experts from among the member states recognised that a system-wide upgrade should take place to allow this unique European research infrastructure to maintain its place as the world leading facility for synchrotron research. An ambitious upgrade programme was proposed and planned in stages to (a) take advantage of latest developments in insertion device and detector technology to provide step changes in the beam quality, brilliance and focusing capability as well as to substantially increase the scope of the experimental stations; (b) construct new long beamlines to enable nanoscale focusing and imaging capabilities for research ranging from materials physics and engineering to biomedical studies; and (c) additional laboratory support facilities to enhance user experiments at the synchrotron end stations and also for sample preparation/characterisation. Planning began in 2006 and the member states approved the project in 2008, to provide this entirely new set of machine capabilities and beamlines to develop new science and technology research opportunities. The first of the planned new beamlines have now become operational and are open to general user access, with user teams from around the EU already accessing some of the unique new opportunities for scientific research. The first phase of the upgrade programme is scheduled to complete in 2015. The ESRF has now proposed to Council a layout for Phase II of the development with a replacement of the storage ring at the heart of the project, and this has been approved to move ahead to a detailed Technical Design Study. The resulting new source will be much brighter than anything currently in operation or planned elsewhere in Europe. It is essential that the UK remain a key collaborator in the construction, development of this unique instrument for scientific research and technology innovation.

In 2002 the UK opened its own 3-G synchrotron source facility, Diamond Light Source (DLS), located on the Harwell/Rutherford-Appleton science campus near Chilton, Didcot adjacent to the ISIS spallation source for neutron scattering. DLS is a remarkable new instrument that takes advantage of the latest advances in ring storage and insertion device technology to achieve extremely high brilliance within a highly stable beam maintained within a diameter of only a few micrometres. The result is an extremely high light intensity delivered to the sample that is comparable to or even exceeds ESRF at energies below approximately 20 keV. Much of the UK attention and budgeting has been concentrated on developing Diamond as a preferred local source for synchrotron research, and that is enhanced by its status as a privately owned company sponsored in part by the Wellcome Trust but mainly by the UK government and research councils. Considerable investments have been made to bring this new facility fully on line, completing beamlines planned throughout Phases I, II and III of its installation. It is hoped that all these beamlines achieve their full projected potential with encouragement from STFC and the user community. However DLS has an inherent limitation for certain classes of experiment because it operates at much lower energy (3 GeV) than ESRF (6 GeV) (primarily due to the smaller size of its storage ring, 561m *vs* 844m). UK user communities accessing Diamond and ESRF cover a very wide range of scientific fields and technological areas and studies carried out at both synchrotron sources are complementary. Experiments fall within three broad classes: (a) those that can be carried out efficiently at Diamond without recourse to the ESRF or other higher energy synchrotron facilities; (b) experiments that can be carried out at DLS but that often also request beamtime at ESRF because of the higher throughput; and (c) those experiments that can only be conducted at ESRF because of the special characteristics of the 6 GeV synchrotron source. The last category encompasses many *in situ* experiments related to materials design and discovery including under extreme physical or chemical conditions, nanoscale focusing and fast tomographic imaging, and specialised light scattering/spectroscopy experiments. The result is that certain experiments that are critical to fundamental research and technology development by UK groups are only feasible at ESRF. For that reason we recommend that the UK maintain its central contribution to the ESRF partnership. That is especially true now that ESRF is moving towards its implementation of a wide new range of beamline facilities with nanoscale imaging and focusing capabilities that are unique in the world.

Appendix 2
A medium-term perspective on the provision of neutrons at the ISIS Facility

The ISIS 1MW idea should be retired. Following the success of TS2 it is clear that it is far more cost effective to invest in target/moderator/instrument optics than in source power. At present, the highest priority is a TS1 target/moderator upgrade, learning the lessons from the TS2 design. This might be combined with some increase to the Linac power (the Linac will need refurbishment anyway) once the technical boundaries are known. This will lead to a performance improvement on TS1 of the order 3 at a cost of approximately £15M – this action is thought to represent excellent value for money. Coupled with instrument investments at the £1M level (*e.g*. TOSCA guide) this will deliver an order of magnitude gain at certain energies on specific instruments. At comparatively modest costs, these initiatives will maintain ISIS's position as a world-leading site for neutron-based science until at least 2025; by which time ESS might be getting into its stride. It would then be possible to develop a longer term proposal for maybe a 2-3MW facility, learning the target lessons from SNS, J-PARC and ESS; and 'decoupled' from any of the existing ISIS hardware. Current views are that the technical optimum is probably a 25Hz short pulse source like at J-PARC. It would be prudent to consider what is the likely scenario for European neutron provision at that point.

Appendix 3
The ESS as a resource for the UK neutron community

Introduction

The European Spallation Source (ESS) is a project for a 5 MW long-pulse spallation source currently under consideration for construction in Lund, Sweden. The current design specifications calls for a neutron pulse length of 2.86 ms, and a single target station with 50 beam ports, with 22 instruments included in the construction budget. The delivery programme (version dated Feb 2012, subject to agreement of the participating Countries) should commence in 2013. The major milestones are: ground break (end of 2013), first building (end of 2015), first neutrons to instruments (2019), full power (2023), completion including the 22 instruments (2025). 3 instruments should be ready to operate in 2019, with an average of 3 instruments/year becoming operational thereafter. This programme timetable is subject to revisions as the design phase progresses, and there are early indications that some delays are likely. The ESS is advertised to provide as much integrated neutron flux as the ILL and 30 times its peak flux in the cold region of the neutron spectrum. Based on the current design, the ESS may have the potential for an upgrade to 50 instruments and 7.5 MW.

ESS performances

The long pulse concept is relatively new and has never been implemented on a large scale. It is therefore difficult to make direct comparisons with existing neutron sources. For most applications, the *peak flux* is the determining factor in setting instrument performances, including the total neutron flux on the sample at a given resolution. Based on this parameter, the ESS at full power will have a significant advantage over the ILL and ISIS TS-I (×30), as well as the SNS and ISIS-TSII (×5-6). The peak flux of the ESS will be similar to that of the new Japanese source J-PARC, once J-PARC runs at the full 1 MW power. However, delivering on these theoretical performances will be far from trivial. The design proposed for the proton accelerator is innovative and in a way over-specified (there is certainly potential for some value engineering), but poses only a moderate risk for the project. Far more critical are the target/moderator package and the instruments, since both rely on untested and challenging designs. Until the full design specifications are known and independently validated, it is safe to assume that the performance parameters are reliable only as an order of magnitude, and that they could be revised downwards by as much as a factor of 2-3.

ESS instruments

The opportunity of building an entirely new suite of instruments at the ESS, starting with a blank sheet of paper, will undoubtedly offer a tremendous opportunity to the development of neutron science and instrumentation. However, the intrinsic characteristics of a long-pulse spallation source are known, and it is relatively easy to predict in broad terms which instruments will offer the best performances and to anticipate some of the difficulties in optimizing and operating them.

The safest neutrons applications at the ESS are those relying on the same designs employed at reactor sources like the ILL. Reactor instruments such as triple-axis spectrometers (TAS) and powder diffractometers could be simply replicated at the ESS. These instruments make limited use of the pulsed structure, and their performances will be comparable to those of ILL instruments. The ESS will not have a hot source, and its performances would be modest if it were to be built. Epithermal neutrons have been crucial to the success of sources such as ISIS, particularly in the field of spectroscopy, but will not be available at ESS based on the current design. Hot TAS (such as IN1) and diffractometers (D3, D9, D4) cannot be built at the ESS. Thermal neutron moderators at the ESS should be bright; however, the close separation between beam ports may require to remove the primary beam shutters and to replace them with sharply bent guides. An extremely careful optics design will be required to preserve full thermal-neutron performances.

Another group of instruments, including low-resolution SANS instruments, low-resolution reflectometers and spin-echo spectrometers, can exploit the long-pulse structure in a rather straightforward way. These instruments can utilise the full length of the pulse and its brilliance and can adopt a rather straightforward design, offering the best prospects for early world-leading performances, provided that the source delivers to specifications. Cold-neutron choppers spectrometers (similar to LET) can also be built at the ESS adopting a rather standard design, and should be able to exploit the full brilliance of the source. However, the lack of high-energy neutrons will severely limit high-energy transfer spectroscopy, a technique that has played a crucial role in the study of strongly correlated systems and quantum magnets.

Medium- and high-resolution diffractometers, SANS and reflectometers are the most difficult to optimize, because the long pulse is too broad to be employed without pulse shaping. This is complex to achieve in the best circumstances, and it is particularly difficult at a 50-port target station with a 5-degree separation between beamlines. The instruments required to exploit a pulse-shaped beam are highly innovative, employing concepts such as wavelength frame multiplication, and could require a long optimization phase. It is noteworthy that successful time-of-flight diffractometers such as GEM, POLARIS and WISH cannot be built to comparable specifications at the ESS: GEM and POLARIS rely on epithermal neutrons for most applications, while the 9 Å frame of WISH is almost impossible to achieve at the ESS.

The ESS has the potential to deliver world-class and potentially world-beating performances as early as 2021 (more realistically, a couple of years later) on a limited range of neutron applications, including low-resolution SANS and reflectometry, cold-neutron spectroscopy and spin echo spectroscopy. Reaching the same level of performances in other fields, including medium-resolution SANS and reflectometry and medium and high-resolution diffraction, may take significantly more time. The ESS will not outperform existing sources in a significant subset of neutron applications; important instruments (e.g., TAS and broad-band diffractometers), based at both reactors and spallation sources, will not be improved or cannot have a direct equivalent at the ESS.

Capital funding of the ESS

A significant fraction of the ESS capital cost (~€1.6B, including 22 instruments) has been pledged by the co-hosts (Sweden and Denmark), with the rest expected from partner countries (as many as 17 have expressed interest so far). 45% of the cash is to be spent centrally and handled by the ESS team, while the remaining 55% representing an in-kind contribution, spent by the partners but “specified” by the ESS. The in-kind model is not new even in the neutron business, and has been previously applied, for example, to fund developments at ISIS. However, its implementation at the ESS on such massive scale raises significant concerns and frankly represents the biggest risk of the whole project. Raising a sufficiently strong and experienced ESS team to coordinate the activities of at least 17 national teams, most of them with little relevant experience in neutron instrumentation, is a daunting task. The risk of balkanisation is well represented by the experience of the APS, where individual beamlines or sectors were not only built but also run by independent groups with little coordination (the APS had subsequently adopted the more centralised ESRF model). In Europe, virtually all the know-how on how to build and operate a modern spallation source is held at ISIS; the negligible involvement of ISIS in the ESS development, in anything other than an advisory capacity is potentially disastrous for the ESS.

ESS and the European neutron landscape

Regardless of its ultimate level of performances, the construction of the ESS will have a profound influence on the European neutron landscape. Its operating budget will approach and possibly exceed that of the ILL and ISIS put together, and such an increase in the overall neutron spending across Europe cannot be justified based on either capacity or capability considerations. Furthermore, no strategy on how to fund operations has so far been announced by the ESS, and most potential partners (including the UK) have a timetable of 2017-2019 to engage in discussions about funding operations. It is therefore almost inevitable that the rise of the ESS will coincide with the demise of some of the other European neutron sources. It is conceivable, for example, that countries operating a national source with equivalent performances to a medium-flux reactor may decide that they would be better served by the ESS, provided that they can gain sufficient access to the instrumentation required by their communities. The big question on everyone's mind is what will happen to the ILL. The ILL convention between the Associates (France, Germany and the UK) expires in 2014, and it is almost certain that it will be renewed for another 10 years. There is a real possibility that a decommissioning plan may be announced after 2024, with major funding for instrumentation upgrades being withdrawn well before this date. It is *imperative* that all European neutron communities (including the UK community) make contingency plans for this scenario. To give a sense of prospective, ESS with 22 instruments would be providing about 16% of current European neutron capacity. If the ILL and other reactors are closed (the intention of Germany to get out of reactors is well known), ISIS may end up as the only place with ability to take up at least some of the lost capacity. Even if ESS could go up to 50 instruments it is incredibly risky to put all your capacity onto a single source.

The UK community and the ESS

The UK neutron community is in a unique position in Europe. In the past 10 years, large investments (~£300M) have been made at ISIS, resulting in the construction of TS2 and of several state-of-the-art instruments on TS1. ISIS is currently the most advanced spallation source in the world, on a par with SNS and J-PARC in terms of raw instrument performances but far superior in terms of scientific productivity. Although instruments such as NIMROD and WISH cannot be built at the ESS, there is an almost perfect overlap between many areas of strength of ISIS-TS2 and of the ESS, and ISIS is currently running much below full capacity. There can be therefore no case, based on either capacity or capability arguments, for the UK ISIS users to migrate their programmes to the ESS until at least the middle of the next decade. Even after 2025, TS2 instrument will remain extremely competitive, while TS1 instruments will be highly complementary to the ESS and will continue to be competitive with SNS, especially if the proposed £7-10M upgrade can realise a ×3 flux increase. The UK community of ILL users is also very strong and productive. The ESS promises the largest gains for some of the applications where the ILL is currently world-best (low-resolution SANS instruments, low-resolution reflectometers and spin-echo spectrometers), and if the ESS programme in these areas is successful, the motivation to migrate would be strong. Should the ILL decommissioning be announced at some point (presumably early in the next decade), many other ILL users will have to look for alternatives, driven by necessity rather than by the prospect of large performance gains. It is imperative that STFC plans for this scenario early on.

Prospects for UK participation in the ESS

The current economic and science funding cycle has significantly reduced the opportunities for capital investments, not only at STFC but also at UK universities. Investments at TS2 have been sustained, with the second tranche of instruments now under construction, and the immediate capital funding priorities *must* be the completion of this programme (which is not yet fully funded), followed by the extremely cost-effective TS1 upgrade (at fixed operating costs) and by further exploitation of TS1 and TS2 beams. Barring a high-level political deal (unlikely but not impossible), there is no reasonable prospect for an immediate UK participation in the ESS construction programme. This is as inevitable as it is lamentable for the prospects of delivering a world-beating neutron source at the ESS early in the next decade, but one has to accept the reality of the situation. From the sidelines, the UK should try to exercise influence and to advise on the design of critical aspects of the project, as well as on the project structure, but realistically there is little prospect for a turn-around on some of the key technical and strategic decisions already taken by the ESS team. Starting from 2017-2019, and conditional to producing a solid business case, the UK may decide to enter negotiations about contributing to the ESS operation. This should be welcome news for the ESS, since it is easy to predict that negotiations with other partners will reach a critical climax around that time, and a new partner with cash to pledge will be virtually impossible to turn down. The level of participation will largely depend on the progress of discussions about the future of the ILL, and on updates on the expected performances of the ESS, which at that point must be fully validated by detailed computer simulations. The UK should fight vigorously for the ILL to be continually funded past 2024 and its instrument portfolio reinvigorated. In this scenario, one could envisage a rather modest UK participation to the ESS (<10%), which will provide access to world-beating instrumentation to researchers in soft-condensed matter, life sciences and high-end cold-neutron spectroscopy, with most of the capacity being provided at ISIS and the ILL. Should the ILL enter in a decommissioning phase after 2024, the UK community will face a capacity and capability crisis, which could be relieved only very partially by a more significant participation to the ESS.

Appendix 4(a)
Laser driven science – overview

1. X-ray FELs are critical to many of the science challenges we have identified. See Appendix-4(c).
2. A need to maintain access to state-of-the-art high brightness IR/THz sources. There is strong potential in security and biomedical applications. A development of the ALICE Facility at Daresbury as a medium-sized user facility supported by other research councils is one possible route that should be considered.
3. Vulcan 10PW is a national priority that will enable a significant number of these high priority Scientific/Technological challenges. It will be a unique facility that will deliver performance unmatched at any user facility in Europe.
4. In general terms, STFC laser facilities plans are for the 10 PetaWatt upgrade for Vulcan to access the ultra-high intensity regime, the DIPOLE programme to access high rep rate lasers using diode pumping (10Hz is expected). Ultimately the combined goal is high power at high rep rate; such a capability opens up a wealth of new possibilities including novel science, where 10Hz enables signal averaging in the regime of ultra-high brightness X-ray and ion sources for applications in materials processing, imaging and medical treatments as well as the long term goal of Inertial Fusion Energy. The 0.1 Hz rep rate Astra Gemini facility is already highly over-subscribed by users
5. Integration of laser technology with Diamond beamlines has started (see Appendix-4(b)) but there is scope for considerable future development, e.g. in time-resolved structure determination.

Appendix 4(b)

Laser driven science – Combining lasers with synchrotron or neutron beamlines

There are already several examples of such collaborations between CLF and Diamond scientists, and the 2011 CLF Annual Report contains an article by Dr Andy Ward (LSF) on cross-facility projects. Examples of current and future plans are given in sub-sections 1-3 below. In addition, the LSF can play a key role by providing facilities for sample testing and pre-analysis in the Research Complex at Harwell (RCaH) building to underpin studies carried out at Diamond and ISIS.

(1). X-ray imaging: There are a number of X-ray imaging beamlines running or being developed. Combining X-ray imaging with laser microscopy has considerable potential to solve real biological questions using X-ray microscopy. Tagging with fluorescent probes allows location of specific molecular species, and this can be combined with the high-resolution imaging that the X-rays will provide. This could be implemented on the cryo-transmission X-ray microscope beamline B24, and/or the soft X-ray microscopy beamline I08.

This "correlative microscopy" approach is currently being used to combine *electron* microscopy with fluorescence microscopy. Doing the same with X-ray microscopy is an obvious next step. There are two ways this could be done. The more complex way is to build fluorescence/laser microscopy capability into the beamline; this is being done on a basic level with conventional wide field imaging, but more sophisticated fluorescence imaging techniques, e.g. confocal, TIRF, super-resolution, could also be implemented. The simpler way is to develop methods for transfer of samples between Diamond beamlines and fluorescent microscopes such as those in the LSF OCTOPUS facility. Samples are imaged on one system and then the same area is re-located with high precision for study by the other imaging method. This approach needs development of special sample stages and image processing software. Developments are on-going in this area in collaboration with Phil Withers and Peter Lee (RCaH residents from Manchester University, EPSRC funded), and will be implemented on the I13 X-ray imaging beamline. There is also involvement with Ian Robinson (UCL, also in RCaH, BBSRC and EPSRC funding).

(2). Time-resolved X-ray spectroscopy and diffraction: The RCaH currently hosts the Dynamic Structural Science Consortium project funded by EPSRC, with PI Paul Raithby (Bath), and involving Mike Towrie of the LSF and Andy Dent and Dave Allan from Diamond..

The consortium project has themes in:

(i) Time resolved single crystal diffraction of small molecule samples (led by Paul Raithby, Bath)

(ii) Time resolved single crystal diffraction of photo-irreversible protein crystals (led by Arwen Pearson, Leeds)

(iii) Time resolved XAFS (lead by John Evans, Southampton).

Mike Towrie (LSF) provides technical advice on laser aspects of the work, and is aiding the consortium to set up RCaH time-resolved diagnostics to prepare for Diamond experiments. The new diagnostics will become part of the RCaH infrastructure. LSF scientists are talking with Diamond beamline scientist about the collection and analysis methodology for TR-XAFS (which uses detectors similar to those on ULTRA).

3. Optical trapping / tweezing / manipulation of samples at Diamond beamlines: The following summarises examples of work by Andy Ward and colleagues from the LSF in bringing optical manipulation techniques to Diamond beamlines.

(i) Diamond Beamline I22 - microfocus for SAXS/WAX: in collaboration with Nick Terrill, the LSF group has built an optical trapping sample environment. This instrument also has simultaneous Raman spectroscopy capability. The first user was Christian Pfrang (Reading) looking at self-assembly within aerosol droplets (Aug 2012).

(ii) Diamond Beamline I24 – MX: the LSF group set-up a UV laser to irradiate a protein crystal in situ on the beamline to stimulate damage.

(iii) Diamond Beamline I24 - MX; (not quite on the beamline but in the room next door to it). The LSF group developed a method for optical loading of microcrystals onto meshes prior to crystallography studies. The initial optical tweezer system has now been replaced by a Zeiss instrument, but the optical sample loader is under continued development.

There are further collaborations at the planning stage, e.g. with Gianfelice Cinque regard optical trapping on the IR beamline (B16), and on using laser tweezers to control crystal orientation and/or rotate crystals in situ. Interaction with soft matter scientists at ISIS has in part been driven through the work of Martin King (RHUL). However, there are problems of use of microscopic samples at the fluxes available in ISIS.

Appendix 4(c)
Laser driven science - Free Electron Lasers (FELs)

X-ray FELs are critical to many of the science challenges that have been identified by this advisory panel: ***Complexity and emergence, Novel materials and Functional materials, Device physics, Warm dense matter, Laboratory Astrophysics and planetary physics, Ultrafast electron dynamics, Structural dynamics of physical systems on all timescales, Fast dynamics/structure studies in biomolecular systems, Imaging cell function at the nanoscale, and Single molecule imaging.*** Moreover there is a strong potential for a large impact on the challenges of life-sciences with the first new protein structure solved using X-ray FEL (combined with emerging nanocrystal techniques) published in Science in November 2012 and the possibility for sub-nanometer imaging of "live" cells published in Nature in 2011. Further it is no accident that two major international laboratories, DESY in Germany and SLAC in the USA, previously famed for high energy physics, have now shifted significant focus to these light sources.

UK X-ray FEL users currently exceed over 50 UK scientists who are active in research at FLASH (DESY), SACLA (Japan) or (the majority) at LCLS (Stanford). This is a growing and very dynamic community. Consultation with this group produced the following recommendations:

(a) A stake in XFEL is seen by all scientists active in this area as the highest priority to ensure this science can grow in the UK.

(b) In the 0-5 year timescale it is essential to establish mechanisms (across the research councils, but with a special emphasis on STFC as it is a facilities issue) to support UK scientists in exploiting the available international opportunities.

(c) In the longer term there must be a review of building a UK based machine (like NLS or of a specification still better matched to future needs).

(d) Continued investment in maintaining the accelerator and light source technology expertise in the UK is essential to retain the option for taking the above step (via Astec, DLS. Cockcroft, John-Adams etc.).

There is an urgent need for the UK scientific community to be provided with sustainable access to fourth generation light sources. The urgency is compounded by the timescale of the major European X-ray FEL (XFEL) due to give first light in 2015. Due to this timescale the UK has perhaps only a limited time window in which to re-engage with the XFEL project on anything close to favourable terms, with the real prospect of being frozen out just as the major results start to flow if we fail to act.

We would therefore recommend that STFC consider the following actions within the period covered by the Programmatic review:

1. Reopen negotiations with XFEL and set aside a realistic budget to make it possible to re-engage. We anticipate that the cash cost can be significantly offset by various in- kind contributions. These include the scheme for the UK to provide R & D for a high power laser to be stationed on a beamline of XFEL through the CLF supported DIPOLE project in association with the Helmholtz Institute. A UK life sciences consortium has also formed and is seeking funding (from appropriate research councils) with a view to fully engaging on the beamline for structural biology at XFEL.

2. Develop the existing efforts at ASTec, DLS, Cockcroft and JAI into a coordinated strategic programme towards next generation FEL technology. This must be done to provide a credible route to allow UK accelerator and light source scientists to participate constructively with the existing FEL projects (including XFEL) as well as providing the strategic underpinning for any eventual based FEL. For instance this may take the form of the development of a FEL test facility to accompany the recently installed electron beam test facility at Daresbury.

Appendix 4(d)

Laser driven science - Medical applications of high power lasers.

As referred to above, high intensity laser plasma interactions can produce beams of charged particles. Most notably a proton beam could be a very compact and precise way of depositing energy in a very localised volume, which is thought to be appropriate for future cancer treatments.

There are other applications too, mainly the use of the laser as a compact accelerator to produce short lived radionucleides for medical treatments. These are otherwise only produced, for example in certain types of fission reactor, and some of these reactors are approaching the end of their lifetimes. An advantage of using lasers to make the nuclides is that short lived radionucleides have to be used close to their source (by definition), which means patients travelling miles when they are probably in a poor state to do so. Laser production via the table top accelerator route has been touted for ages.

Compact, rep rate laser technology (which DiPOLE is prototyping an early stage of) will transform an observed phenomenon in a big laser facility into a source in a hospital basement.

Appendix 5

Heritage science.

The heritage area is not one that the UK takes seriously, compared to our European neighbours. There are sporadic initiatives (e.g. EPSRC/AHRC in 2009) but there is never anything on-going. The facilities have a growing role to play in this area – particularly in the use of microfocus techniques. It is interesting to note that in many cases, e.g. Soleil, there is a specialist unit for heritage proposals (senior scientist and post-doc). This is essential to act as an interface between the heritage (cultural, museum, conservator, etc.) specialist and the scientific expert. ISIS/Diamond could do with this sort of approach. There are some good groups in the UK but they are not coordinated. Unfortunately, the economic benefits will be small. But man cannot live by bread alone!

Appendix 6

Research Council interfaces

There are serious concerns on the limited number of postgraduate studentships currently available in academia since the decision of the EPSRC not to support project studentships. Few of the current crop of DTCs have inherent links to Central Facilities (CF) and it is suggested that, should this situation continue, then there will be a scarcity of postgraduate students to undertake the exciting and relevant work outlined above. Furthermore, it will lead to a paucity of trained scientists to feed in to the pool of next-generation users. Without a strong user-base, the facilities will under-perform and not achieve their full potential; thereby hindering the progress of UK Plc in this knowledge-driven economy. It is suggested that RCUK considers supporting studentships for projects that have strong connectivity to CF-related activities. This would provide an excellent opportunity for a joint STFC-EPSRC initiative and would represent tangible evidence of ‘joined up thinking’ within RCUK.

Appendix 7

Universities as direct stake-holders in Central Facilities

Academic researchers from science departments from UK universities are major users of Central Facilities (CF). This grouping undertakes the work and the training of new scientists in areas of endeavour that strongly connect with the goals and targets of RCUK. However, the funding landscape, as seen for a university perspective, is asymmetric. Whereas EPSRC and BBSRC provide Full Economic Costing (FEC) with their grants, UK academics using CFs via STFC schemes such as Direct Access or Programme Access (or equivalents) do not receive FEC. Consequently, UK university managements have less incentive to encourage new academics to engage in medium-term workplans at CFs, as they do not return FEC to the academic institution. In the long term, wider use of CFs by UK academics could be stimulated by allocating a FEC component within beamtime awards. Such a scenario would give the UK universities a greater stake holder role in CF-driven science.