BASIC ENERGY SCIENCES ADVISORY COMMITTEE
to the
U.S. DEPARTMENT OF ENERGY

PUBLIC MEETING MINUTES

FEBRUARY 11 - 12, 2016

Bethesda North Marriott Hotel and Conference Center
5701 Marinelli Road, North Bethesda, MD 20852

February 11 - 12, 2016
DOE BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened on Tuesday and Wednesday, February 11 - 12, 2016, at the North Bethesda Marriot Hotel and Conference Center in North Bethesda, MD, by BESAC Chair John Hemminger. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Attendees can visit http://science.energy.gov/bes/besac/ to learn about BESAC and download the meeting presentations.

Committee members present:

John Hemminger, Chair	Roger French	Mark Ratner
Simon Bare	Bruce Gates	Anthony Rollett
Dawn Bonnell	Ernie Hall	Frances Ross
Gordon Brown	Sharon Hammes-Schiffer	Gary Rubloff
Sylvia Ceyer	Bruce Kay	Esther Takeuchi
Yet-Ming Chiang	Stephen Leone	Douglas Tobias
Sue Clark	William McCurdy, Jr.	John Tranquada
Beatriz Roldan Cuenya	Monica Olvera de la Cruz	
Persis Drell	Philippe Piot	

BESAC Designated Federal Officer:
Harriet Kung, DOE Associate Director of Science for Basic Energy Sciences (BES)

Committee Manager:
Katie Runkles, DOE BES

THURSDAY, FEBRUARY 11, 2016

WELCOME AND INTRODUCTION

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) was convened at 8:20 a.m. EST on Thursday, February 11, 2016, at the Bethesda North Marriott Hotel and Conference Center by BESAC Chair **Dr. John Hemminger**. Committee members introduced themselves and Hemminger reviewed the agenda.

NEWS FROM THE DOE OFFICE OF SCIENCE

Dr. Cherry Murray, DOE, Director of the Office of Science (SC), reviewed the FY16 budget and the FY17 Request. Dr. Murray's FY17 priorities include maintaining strong support for discovery science and world class research facilities, supporting science for clean energy, fostering relationships with Congress and research partners, and implementing best practices in lab management.

SC requested $100M in new funding for FY17 across four programs. Another $100M in mandatory funding is requested for investments in university research in all programs. Murray described specific activities in each program's budget request and pointed out correlations between the other programs and the SC Basic Energy Sciences (BES) Program. BES issued a funding opportunity for new Energy Frontier Research Centers (EFRCs) in FY16 and plans another for FY17.

Discussion

Tony Rollett asked about benchmarking U.S. accelerator scientific achievement and user facilities against other countries. **Murray** noted that the U.S. is slipping behind and needs to maintain world-class status. The current budget is good, but an increase is not expected. SC must evaluate and prioritize facilities to sunset those that are underperforming.

Murray described for **Monica Olvera de la Cruz** facility partnerships with the National Science Foundation (NSF) on the Large Synoptic Survey Telescope (LSST) and the Long-Baseline Neutrino Facility (LBNF) Deep Underground Neutrino Experiment (DUNE), as well as an agreement with CERN for LBNF DUNE. Discussions are being held with MEXT (Ministry of Education, Culture, Sports, Science and Technology) in Japan to collaborate on projects, and with the National Institutes of Health (NIH) on bioimaging facility needs. Genomics and the Human Genome Project are activities with big data sets that can benefit from exascale computing.

Beatriz Roldan Cuenya asked whether the international collaborations were at the facilities level or at the research level. **Murray** shared that this differs by program. For example, in SC High-Energy Physics (HEP) and Fusion Energy Sciences (FES), the facilities are so expensive that they need to be international collaborations; however we also fund researchers to conduct experiments at the Large Hadron Collider, for example. BES has tried to coordinate funding opportunities with partners and it has been difficult. It is easier to develop relationships in the context of facilities.

Harriet Kung added that BES is in the early stage of exploring EFRC exchange of foreign staff from countries that have bilateral agreements with DOE.

Hemminger asked about the interactions within the SC Programs, specifically how to ensure important areas of science are not lost when programs are refocused. **Murray** called this an easy management issue as it is within the SC programs. Lab planning is jointly done by the programs, and discrepancies are identified for reconciliation. In 2016, this activity will include the DOE energy programs and there are things that fall between SC and energy programs. Cross-cut activities can address gaps, and this is something that the Office of Management and Budget (OMB) likes to see.

Bruce Gates asked if BES' nature is changing to become less basic, broader and more applied. **Murray** responded no to all characteristics but indicated that things may become broader. Discovery research is very important and represents two-thirds of the portfolio. DOE is a mission agency and the research it supports has to inform energy or national security needs.

Murray confirmed for **Simon Bare** that the university grants requested in the Presidential budget is a one-time activity supported by mandatory funds. The current budget caps set by Congress are too low, and the request seeks mandatory authority for this activity.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE, Director of Science for BES, shared staffing changes in BES to include the additions of **Joshua Haines** as a Science Assistant and **James Rustad** as the new program manager for Geosciences.

The FY16 Consolidated Appropriations Act appropriated $1,849M for BES, an increase of $115.8M over FY15. Appropriations and funding request history shows an increase of more than 50 percent since FY00. The growth from FY15 to FY16 is the largest increase since FY 2009 and the first time planning level and appropriation came close in many years. Kung noted that BES is improving how it structures its requests to respond to the mission and community needs.

User facilities usage dropped in FY15 mostly due to the closing of National Synchrotron Light Source (NSLS). Funding increases in FY16 should allow for optimal user support.

Three computational materials sciences awards totaling $8M were made in FY15. Funded research will support the Materials Genome Initiative for Global Competitiveness and provide software usable by the public and private sector communities.

The FY16 Computational Materials Sciences FOA has been announced and will focus on materials and software not supported by the FY15 awards. The EFRC solicitation for FY16 was also announced and will support multi-disciplinary research challenges in areas relevant to environmental management.

The Sustainable Ammonia Synthesis Roundtable will be held on February 18 to deliver a report that will inform BES planning for this area of research.

The FY17 budget request is $1,937M representing an increase of $88M over FY16. An increase in funding of $52M for core research is one highlight.

Kung reviewed changes in construction/Major Items of Equipment (MIE) funding from FY00 to FY17.

The FY17 request was informed by the Quadrennial Technology Review (QTR) and the BESAC report "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." The QTR is being furthered by cross-cutting working groups with membership from across DOE.

For the FY17 request, BES identified energy efficiency and extreme environments as core research areas that enable mission innovation. Quantum materials is another area for growth in the FY17 request. The goal is to identify new materials for next generation semiconductors, energy efficient electronics, and technological advances for energy technologies.

Advancing the imaging of geophysical and geochemical signals in the subsurface is a grand challenge identified by a subsurface roundtable. BES proposes a new group of EFRCs to address the grand challenge. Accomplishments in this area can drive greater energy return from subsurface sources and the understanding of geological response to energy production activities at the subsurface.

There is a critical need to increase computational chemical sciences research, and the development of open source software in particular. In FY17, BES will request new funding in this area. There has been tremendous improvement in the past decade but handling more complex phenomena requires better methodology and software.

BES prepared a new brochure describing changes in the BES program in FY 2015 and accessible research highlights.

The "Neuromorphic Computing Roundtable: From Materials to Systems Architecture" was held in October 2015.

Kung announced upcoming Basic Research Needs workshops for 2016.

BESAC has been presented with a new charge to prioritize facility upgrades.

Discussion

Bill McCurdy asked about the mission innovation funding and its origin. **Murray** shared that mission innovation was announced by 20 countries at the beginning of the United Nations Climate Change Conference 2015 (COP21). They pledged to double their clean energy research budget in five years. In 2016, SC set a funding baseline. Multiple DOE offices are addressing this with funding set at $4.8B for FY17.

Yet-Ming Chiang asked if mission innovation will represent a change in metrics for success. **Murray** shared that the new activities that will go into mission innovation are supposed to be high-risk, long-term, and high-reward. DOE Secretary Moniz requested that research efforts be investable, allowing for private sector engagement and support.

Kung shared with **Gordon Brown** that she is unaware of funding from DOE Environmental Management for basic research but noted BES' commitment to this important area. It is proposed that EM support more applied research and they have $50M to $60M in funding to scale-up transformative research that comes out of SC.

Kung clarified for **Steve Leone** that the role of roundtables is to provide a quick study at a smaller scale on specific topics.

Philippe Piot asked about BES input on accelerator technology. **Kung** shared that a group of program managers from multiple programs set priorities and are developing critical needs based on input from accelerator program customers. The BES R&D budget for accelerators and detectors is small and the group is focused on advancing technologies for the future.

Gates asked about the Congressional language on ammonia synthesis. **Kung** shared that it appeared in the appropriation language but the source is not known.

UPDATE ON THE REPORT "CHALLENGES AT THE FRONTIER OF MATTER AND ENERGY: TRANSFORMATIVE OPPORTUNITIES FOR DISCOVERY SCIENCE"

John Sarrao shared the report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." It was published in November 2015.

The scientific, funding and programmatic landscapes have changed significantly since 2007 when the BESAC Grand Challenges report was completed. Transformative opportunities have emerged that build on standard discoveries and not just eureka-type discoveries. These are crosscutting opportunities. The importance of tools is clear.

There are five transformative opportunities described in the report. Each represents an opportunity and challenge. Each has roots in the set of challenges from 2007. The report emphasizes the importance of each opportunity and actions that could fulfill each opportunity.

There are three areas identified for enabling success: synthesis, instrumentation and tools, and human capital. Synthesis is an important domain for fulfilling the opportunities with two aspects: knowing what to make and knowing how to make it. Advances in instrumentation and tools are needed to support discovery in complex systems and drive progress. Tool development must be part of the funding mix to help research reach its full potential. In the past, there has been insufficient focus on developing skilled tool builders. Human capital is another important domain. BES is committed to building the current and future workforce, and they must be brought into a balanced investment portfolio.

The challenges from 2007 are still valid and provide roots for redoubling those efforts through investments in the new set of transformative opportunities.

Discussion

None

NEWS FROM THE OFFICE OF ADVANCED SCIENTIFIC COMPUTING RESEARCH

Steve Binkley, Director, Office of Advanced Scientific Computing Research (ASCR), shared that ASCR's origins date back to the Manhattan Project. Computer science is now recognized as a discipline and it is part of DOE's portfolio. Atomic energy laboratories were among the first to use supercomputers.

Computational and networking capabilities supported by ASCR seek to extend the frontiers of science and technology. Binkley described five areas of ASCR support, and expanded on scholarship support through the Computational Sciences Graduate Fellowship.

ASCR is developing plans for new computing technologies, in conjunction with large computing companies such as IBM. ASCR operates three large computing facilities and is driving to advance computational power up to 200 petaflops.

Optimizing DOE's scientific performance requires linking all DOE sites together through the Energy Sciences Network (ESnet). It has 100 gigabits of capacity as its backbone. A similar network system called Internet2 connects universities and is supported by NSF. The two systems work together. ESnet is constantly being upgraded with research being done in a number of areas.

There is significant interest from U.S. high-tech manufacturers in high-performance computing (HPC). Transportation and modern electronics are two fields generating interest.

A review of computational requirements looks at opportunities and challenges across SC to mesh computational capabilities with science needs and informs ASCR's future direction.

Structured workshops also provide direction. Workshops unite scientists and ASCR-community individuals to discuss opportunities and challenges over the next five years, and to collect details about the scientific needs and opportunities within specific programs.

The Scientific Discovery through Advanced Computing (SciDAC) program has become a pathway for outreach from ASCR to the science community. SciDAC partnerships coordinate computer science/applied math researchers with researchers who are advancing the codes in their research domain. The program is in its third five-year cycle, with 18 partnerships across SC programs. SciDAC will next engage programs to help construct the next round of SciDAC partnerships.

ASCR invests in exascale computing. It is possible to get more transistors on computer chips. Computational advances will rely on harnessing this count over the inability to advance clock speed. Extreme scale computing is the focus of DOE's exascale computing initiative. ASCR is partnering with the National Nuclear Security Administration to jointly advance hardware, software, applications, large data, with applied math and computing science underpinnings.

DOE's overall exascale program has several components. The Exascale Computing Initiative (ECI) and the Exascale Computing Program (ECP) strive to meet goals that include 20 pJ per average operations, greater concurrency, and an effective application development ecosystem.

The community is a resource for potential exascale applications. In 2015, 17 DOE laboratories provided responses. This preceded a request for information from NIH, NSF, DOE, academia, and national labs to identify opportunity areas for exascale computing. Biology, physics, and mathematical sciences were the three fields with the most responses.

Binkley shared data on the shift from giga-level computing to peta and exa, identifying the need for software advances to keep pace with transistor and hardware advances. Advances in

software are being jointly supported by BES and ASCR. Both programs made FY15 awards to advance software and hardware development.

The Exascale Initiative is being projectized to follow DOE's established process for review and decision protocols. Binkley projects a critical decision (CD) process starting with CD-0 in 2016 leading to CD-4 by 2026. So far, DOE has kept more than one technology option available to leverage advances as they become known.

Extreme-scale science generates huge amounts of data. Large bodies of knowledge and data exist within the National Energy Research Scientific Computing Center (NERSC) systems. ASCR studied the data requirements across various programs, and identified data quantities and rates. As an example, the study pointed out the level of computing being used to crunch data from the Linac Coherent Light Source (LCLS).

Neuromorphic computing is an area of joint interest by ASCR and BES. DOE produced a report in 2015 that identifies research directions, specifically describing the value and potential impacts of neuromorphic computing.

Discussion

Binkley told **Doug Tobias** that several codes are currently available for scaling across the current leadership class of computers. Conspicuously absent are materials science and chemical science codes. ASCR reviews proposals that often suggest scalability levels of hundreds of thousands of cores. More research can be done in this area. More collaboration between computing and physical scientists is needed.

Cuenya noted recent areas of collaboration and asked about new computational capabilities that could support electrocatalysis. **Binkley** suggested that this should be further explored. A meaningful subset of catalytic systems is essential. Software is needed for this area.

McCurdy asked if BES should be more involved in the underlying physics of computing, as physics and scientific issues that drive quantum computing advances are in the SC portfolio. **Binkley** shared that skepticism that quantum computing could deliver results existed until recently. There have been many advances in the last seven years. It has not been obvious to agencies that it is close enough for people to get sufficiently excited and invest in it. An inter-agency working group noted that quantum computing is nearing a tipping point and opportunity to do something in the next few years may emerge. Slow and steady investing is the right pace for now.

Roger French described computing usage by his group. A cultural struggle exists between those focused on big flops and others focused on data. **Binkley** described the goal ratio between bytes and flops. Memory can be more expensive with each step in technology. One advance making its way into large computers is non-volatile random access memory. This gets at the energy problem because it takes less energy. There may be more algorithms that get into large memory applications. **Binkley** described the benefits of ARM chips. He expects advances with the Church-Turing Model of computing in the next decade.

NEWS FROM THE OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH

Dr. Sharlene Weatherwax, Director, SC Office of Biological and Environmental Research (BER), shared BER's focus on complex biological, climate, and environment systems. Its work ranges from single microbes to global-scale systems.

BER is set-up to manage research and user facilities in two divisions: Biological Systems Science, and Climate and Environmental Science.

Foundational science supported by BER explores observational and experimental capabilities with modeling. Predictive understanding comes from computer-based modeling, in areas such as genome-enabled biology and the understanding of the effects of greenhouse gas emissions.

There are three BER scientific user facilities. The Joint Genome Institute addresses genomic sequencing needs. The Atmospheric Radiation Measurement Climate Research Facility takes field measurements and provides data products to inform cloud and aerosol science. The Environmental Molecular Sciences Laboratory does research on aerosol chemistry, biological systems, geo- and biochemistry, and interfacial and surface science.

The Bioenergy Research Centers started in 2007 were grounded in basic research but had milestones and deliverables. There are three centers with public and private sector partners. The funding renewal period will end in FY17. Future funding is sought to advance the movement of research findings to industry. A competitive FOA will be announced soon.

Many BER programs strive to develop enabling technologies to perform systems biology. This is where BER interacts with other SC programs and agencies. The DOE Systems Biology Knowledgebase (KBase) is a foundation to technological advances.

DOE has focused on climate change research since the 1950s. Atmospheric transport is addressed through general research into system components, how they are changing, and how the climate is changing as a whole. BER relies on ASCR facilities to help manage data. Modeling is used to understand the human impact on environmental conditions and changes.

Some of the oldest climate code used in computing deals only with atmosphere. Increased climate model sophistication drives code development to leverage the latest machines. The Accelerated Climate Model for Energy (ACME) is a multi-laboratory project that is developing a climate model that runs at a high level of resolution and assimilates all of the climate data available.

Sensor systems give observations (data) that is incorporated into models. Regions chosen for data collection are globally important, sensitive to climate change, and understudied in predictive models. BER research is being conducted through the Next-Generation Ecosystem Experiments.

BER funding is available through grants to academia and private institutions, and through integrated team funding opportunities at DOE laboratories in scientific focus areas.

Community input gives BER strategic direction and informs FOAs. Input comes from community meetings, BER workshops, and other organizations.

Instrumentation development at user facilities, joint user facility calls that leverage cross-program capabilities, mutual participation in PI meetings, and joint workshops on interface topics are all opportunities for cross-collaboration between BER and BES. The Kbase can also be an asset to BES programs as they conduct data analysis and integration.

There is a cross-facility and cross-discipline call to conduct research at BER scientific user facilities. An example in FY16 is a pilot program at the Environmental Molecular Sciences Laboratory (EMSL) and the Atmospheric Radiation Measurement Climate Research Facility (ARM) researching atmospheric aerosol science. There is a single review of proposals for access to both facilities.

BER is supporting the Brain Research through Advancing Innovative Neurotechnologies (BRAIN) Initiative to aid understanding of the human brain. BER can provide specialized technologies to support research such as high resolution tools or molecular nanoprobes. A joint workshop in the fall of 2015 defined scope of DOE participation. Additional workshops are planned for more specificity.

Discussion

Ernie Hall noted that BER's research portfolio is globally-oriented and asked about international collaboration. **Weatherwax** described how BER benefits from data sets created in other countries and others' projects. The Go Amazon campaign in Brazil is an example wherein partners can plan their timelines to help one another. Genomics is another area with international focus. For example, we might sequence plants that aren't native to the U.S. or grown here.

Weatherwax told **Brown** that funding for research into contaminant fate and transport still exists. EMSL is an example where research into contaminated species is being done. There was a prior push to narrowly study certain contaminants. Now, BER looks at biogeochemistry and all critical aspects are put into a modeling framework.

Hemminger added that a lack of fundamental science in more complex global models can cause parameters to be tweaked and may push the results off the map. A lack of fundamental chemistry knowledge can be dangerous in a systems-oriented approach. He suggested that BER is doing less of this now. **Weatherwax** shared that the challenge is in how one moves upscale. A key question is when to parametrize and roll things into a black box, and if usable information can still be produced. BER deals with this topic often and works to bridge across models and across scales, and has addressed this in workshops. There is emphasis on understanding how components fit onto models. The three BER research centers look at components, but the emphasis in BER is how things fit into a bigger context.

Gary Rubloff asked about spinoffs of genomics research to biomedical applications such as the microbiome. **Weatherwax** shared that many BER tools have cross-utility, and are applicable to microbiology and applications. There is a specific request in FY17 to address the microbiome, to understand how microbes work together and how they are relevant to human health.

Weatherwax described for **Gates** the status of biofuels. The price of oil was much higher when this research began. BER wants to overcome the challenges inherent in producing biofuels, and it is not just a price point challenge. BER has learned a lot about fundamentals, including how to use switchgrass and make targeted changes to generate more fuel. There are interesting spinoffs. Some tools have broad application beyond biofuels.

REPORT ON THE BASIC RESEARCH NEEDS FOR ENVIRONMENTAL MANAGEMENT WORKSHOP

Sue Clark of Pacific Northwest National Laboratory and Washington State University described the Basic Research Needs for Environmental Management Workshop. It was sponsored by BES, BER and ASCR, and held in July 2015.

Since 1989, Environmental Management (EM) has cleaned up 91 of 107 sites from the nuclear weapons legacy. The remaining sites present considerable challenges. Challenges include maintaining a skilled workforce able to address these issues over the next 50 years. To date, $152B has been spent and it is expected that $235B through 2065 to finish the clean-up mission. The current budget demonstrates a $28B gap in funding between the historical budget level and the cost estimate profile for what is needed.

The high-level radioactive waste and chemistry at sites that require cleanup present unique challenges that seem counterintuitive. This contributes to taking more time and funding than expected to ensure successful clean up.

A task force of the Secretary of Energy Advisory Board gave recommendations in 2014 for effective environmental management to include creating a fundamental research program to develop new knowledge and capabilities to address the EM challenges.

The interrogation of inaccessible environments over extremes of time and space is one challenge identified at the workshop. Innovations are needed to overcome the challenge of accessing and understanding structures, waste forms, and environmental contamination.

Understanding and exploiting interfacial phenomena in extreme environments is a second challenge. There are unprecedented extremes in complexity, harshness, space, and time. Advances could aid understanding of interfacial phenomena in extreme environments, and how in heterogeneous environments they dictate system properties and functionality.

Incredible advances are being made in science, computing and imaging, but the environmental part of DOE has not necessarily benefitted from these advances.

The workshop identified six priority research directions as well as cross-cut areas of ex situ and in situ characterization and simulation.

Discussion

Gates asked about examples of basic research successes that have led to environmental remediation success. **Clark** noted that work at Oak Ridge National Laboratory has enabled the removal of cesium and strontium from waste. Chromium (III) research in high level waste informs the processing of waste streams today.

Rollett asked about the extent to which the community is using 3D imaging. **Clark** shared that the need for mesoscale imaging resonated through everything that workshop participants described. Phenomenal advances in imaging will provide excellent tools to achieve things that could not be accomplished ten years ago.

DISCUSSION OF THE CHARGE TO BESAC TO PRIORITIZE FACILITY UPGRADES

John Hemminger described the charge to BESAC issued by Dr. Cherry Murray, Director, SC. The charge calls for BESAC to update the prioritization for the next 3-4 facility upgrade projects in the BES portfolio. The subcommittee will consider two criteria in the prioritization: ability to contribute to world-leading science and readiness to proceed to construction.

UPDATE ON THE LCLS-II HIGH ENERGY UPGRADE

Chi-Chang Kao, Director of SLAC, described the proposed Linac Coherent Light Source-II High Energy (LCLS-II-HE) upgrade to move the spectral range to 12 keV and above. The upgrade would contribute to the challenges and opportunities outlined in the report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science."

LCLS exposed new directions in research across multiple disciplines and highlighted key areas where coherence, femtosecond time-resolution, and high pulse energy can make an impact.

LCLS-II fulfilled BESAC recommendations made in 2013 by producing a high repetition rate. The HE upgrade would extend the high rep rate to high energy to deliver higher photon energies. This would exceed any existing or proposed x-ray capabilities worldwide.

The upgrade would double the electron energy of the accelerator, install a second bypass line, and include new instruments. It would add 19 cryomodules to extend accelerator performance to 8 GeV. A bypass line would enable a dual electron-beam capability, allowing parallel or combined beam experiments. New instrumentation will leverage the transformative nature of the new source. The upgrade would occur in existing infrastructure.

With the upgrade, structural dynamics at the atomic scale could be studied. The correlation of catalytic reactivity and structure could be studied by understanding coupled electronic and nuclear dynamics. There is also opportunity to investigate emergent phenomena in complex

materials with the planned energy resolution of 1 meV. Another possible outcome is the ability to image the diffusion and fluctuation of material structures to enhance understanding of these processes in the real world.

Kao described LCLS-II's readiness to proceed. Existing proven technology can be leveraged. Cryomodules are already in production for LCLS-II, so this upgrade would utilize the established the supply chain. The upgrade would use the existing tunnel and sufficient cryogenic capacity will be available. With LCLS-II, an experienced team and integrated management system are already in place.

Discussion

Chang described for **Gates** the status of international competition. The real competition is based in Europe (EuXFEL) which is also using a superconducting linac that allows them to reach high energy.

John Tranquada asked about the need for higher field gradient. **Chang** clarified that the project assumed a conservative field gradient but testing is showing higher performance. They assume that cryomodule performance will be comparable for the proposed upgrade and hence the performance will be achievable within the existing tunnel.

Chang described the LCLS-II-HE bypass line to **Hemminger**. They would have flexibility to hit whatever resonance experiments need. EuXFEL won't have this flexibility.

UPDATE ON THE ADVANCED LIGHT SOURCE UPGRADE

Mike Witherell, Director, Lawrence Berkeley National Laboratory (LBNL), and **Roger Falcone**, Director, LBNL Advanced Light Source (ALS) described the ALS upgrade (ALS-U).

The ALS uses coherent, soft x-rays and advanced spectromicroscopies to meet BES grand challenges. The upgrade concept will add an accumulator ring to the existing storage ring, reuse the beamlines and infrastructure, and install multibend-achromat (MBA) storage ring technology. Diffraction-limited beams can be enabled by MBA. That is currently being implemented in Sweden and is performing very well.

ALS-U would be optimized to provide the highest coherent soft x-ray flux, exceeding any current or planned facility worldwide. A benefit is accessing elemental resonances to help identify atoms, molecules and chemical states.

The ALS-U concept includes leveraging the existing infrastructure and the use of MBA technology, surpassing existing and planned soft x-ray sources.

Coherence enables dynamic imaging with higher spatial and temporal resolution. Supercomputing performance will be needed to manage this higher rate of data taking.

Falcone described three examples that are possible through ALS-U that meet challenges identified by the BESAC report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science."

The cost for the upgrade is $300M and includes escalation, contingency, and assumes an FY16 start date. Ring replacement will take six years with 10 to 12 months of dark time.

Discussion

Hemminger asked about the upgrade of optics for existing beamlines and if there would be beam damage to existing optics. **Falcone** shared that the real issue is preserving coherence. To avoid this issue, capabilities have been explored with vendors.

Falcone described for **Hemminger** that APS-U and ALS-U crossover on the flux curve around 3 keV.

Tranquada asked about detectors. **Falcone** shared that they are developing detectors for high-speed read-out. Detectors that operate at a few hundred hertz are available now. They are working on kilohertz detectors

Olvera asked about interactions with NIH and the BRAIN initiative. **Falcone** told BESAC that discussions are being held with the community to understand how biosciences can take advantage of the proposed upgrades.

Piot asked about brightness. **Falcone** described that the facility would follow the existing brightness curve, with ALS-U reaching 10^{22} in brightness.

Cuenya asked why the upgrade will take around six years with up to 12 months dark time, how ALS-U will be positioned globally, and about the chances that more than one DOE facility would be simultaneously dark. **Falcone** believes that DOE would never have more than one light source down at a time. ALS is building techniques and beamlines that are ALS-U-ready to reduce project length and dark time. Building up these capabilities would hopefully reduce the build time and dark time. This amount of dark time is consistent with these types of upgrades.

Rollett asked if the upgrade proposed is aggressive. **Falcone** clarified that it is aggressive but he does not believe that there is technical risk due to what is currently demonstrated.

REPORT ON THE ADVANCED PHOTON SOURCE UPGRADE

Peter Littlewood, Director, Argonne National Laboratory (ANL), described the Advanced Photon Source-Upgrade (APS-U). It would be the world's leading next-generation facility for high-brightness hard x-rays. The capability of current storage rings will be exceeded by two to three orders of magnitude in brightness, coherent flux, and nano-focused flux.

The APS-U will consist of a 6 GeV MBA lattice in the existing tunnel, use new and upgraded beamlines, and use new insertion devices in order to fulfill the BESAC vision presented in 2013.

Compared to other light sources and present designs, the APS-U will exceed the ESRF-II and SP8-II. Data on some other light sources such as work in China are unknown. The APS-U represents the ultimate 3D microscope to map any atom's position, identity and dynamics. Workshops and publications over the previous decade have made the science case for the upgrade.

Littlewood told BESAC how the APS-U will meet challenges in its report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science."

Costs for the upgrade have been vetted and are comparable to recent projects of this scope.

The beamline planning process for APS-U will be complete this summer. White papers were received for new or upgraded beamlines. Papers represent more than 200 institutional partners.

CD-1 is complete. CD-2 is expected between FY16 and FY17. The goal is to have the full complement of beamlines when the project is complete. APS has a fully-staffed upgrade implementation team.

DOE reviews have validated readiness for the upgrade and R&D for prototyping has been progressing. Littlewood noted that the community is behind the effort.

Discussion

Rollett noted the remarks on instrumentation and how integration of computation with the beamlines is important. He asked about observations on how the user community is shifting. **Littlewood** shared that white papers demonstrate interest in coherence and imaging. In

particular, there is a shift from protein crystallography to areas such as biological imaging. The community can grow in different ways through APS-U capabilities.

Hemminger asked about end stations capable of using APS-U, noting that instrumentation and staffing is also important. **Littlewood** shared that the issue is that one can take the data but cannot look at it long enough to extract value. ANL is working on ensuring computing capability to make this possible.

Hemminger asked about white papers down selection. **Littlewood** proposed that the ANL would like to include 6 new beamlines and 2 upgraded beamlines by CD-2.

Mark Ratner asked if hard x-rays would cause soft, biological samples to blow apart. **Littlewood** explained that ptychographic imaging requires photons to go straight through the sample. Hard x-rays are better than soft x-rays for this purpose.

Littlewood told **Gates** how end stations or beamlines are changing to do more in operando experiments. APS engages the community to look at what other instrumentation is needed on beamlines such as lasers. APS will continue progress to install for example an MBE growth facility at the end of a beamline. Focusing and optics are needed to deliver the beam to the sample.

Littlewood told **Gates** that the APS-U operating budget should be at about its current level. There will be 60 operating beamlines as there are now. The staff would need to be maintained to support this. There would be continuing progress to introduce upgraded beamlines in advance of APS-U project.

Littlewood confirmed for **Brown** that all 60 beamlines would be operating at the end of the project.

Littlewood told **Brown** that collaboration access teams are being engaged one-by-one.

PRESENTATION OF NEXT STEPS IN PRIORITIZING FACILITY UPGRADES

Hemminger shared that a subcommittee will guide prioritization deliberations. It is hoped that there will be international, BESAC, and community representation on the subcommittee

A meeting in April will lead to a report to be presented at the BESAC meeting in June 2016.

NEWS FROM THE UNDER SECRETARY FOR SCIENCE AND ENERGY

Lynn Orr, Under Secretary for Science and Energy, acknowledged the value of the independent voice of BESAC in communicating scientific needs and interests to elected officials.

The United Nations Climate Change Conference (COP21) negotiations held in Paris in 2015 were an influence on the President's FY17 budget request. Countries' declarations of the climate change research and actions that they could implement by mid-century were a helpful pre-text to COP21.

20 countries announced their commitment to double their clean energy efforts over five years. The nations will meet in San Francisco in June 2016 to discuss their progress.

The budget act passed in December 2015 provided generous increases in FY16 but was flat in FY17. Coming out ahead indicates that the President and OMB see the importance of DOE research, from discovery science to use-inspired EFRCs to fundamental work that enables progress across the R&D space. Catalysis research and advances are an example and highlights the potential for DOE's efforts.

The 2013 BESAC report on light sources has given DOE the sense of the potential possible and impacts on energy, science and society. It has empowered DOE with the ability to tell elected officials that the science community has come together to identify research aims. The

new BESAC report on transformational opportunities is just the advice we need for transformative breakthroughs with potential impact on science and society.

BESAC is now charged to prioritize facility upgrades. The response to the charge is important to the DOE and the community at large. It will help lay out the plan for the next decade.

Discussion

Orr responded to **Gates'** concern about facility construction costs, noting that no single agency or country can afford building a single large facility. CERN is an example of the need for collaboration. Cost and opportunity drive decisions. Other nations envy the U.S.' laboratory and scientific structure. As they build their approaches, the U.S. should be involved. Involvement should bubble-up and not just be top-down. Most efforts will be driven by bi-lateral agreements.

Orr responded to **Hemminger's** interest in the mandatory spending included in the President's budget request. The transportation initiative is one source of funds for the mandatory spending proposal. It is supported by the proposed $10 per barrel fee on crude oil. Clean-up of old uranium and plutonium processing sites is another mandatory spending example with an identified funding source. Oil and gas royalties could contribute as well.

Cuenya asked about Congress' funding of ammonia synthesis. **Orr** is unsure where this came from. DOE discusses resource allocations and there are more ideas than there are funds. The budget request is developed through negotiations with OMB, then it goes off to Capitol Hill. Congress can have ideas that can differ from the President's Budget.

Orr told **Rollett** that he is unaware of Congress's recommendation that agencies spend one percent of their R&D budgets in each state. There is a 0.9 percent tax on energy R&D money for commercialization. It is about $20M this year.

PUBLIC COMMENT

None

ADJOURNMENT

The meeting was adjourned by **Hemminger** at 5:05 p.m.

FRIDAY, FEBRUARY 12, 2016

The BESAC meeting was convened by **Chair John Hemminger** at 8:00 a.m. EST.

PRESENTATION ON THE USER FACILITY COMMITTEE OF VISITORS

Jim Murphy, Director, BES Scientific User Facilities Division (SUFD), described the BES SUFD Committee of Visitors (COV). The SUFD COV is held every three years and this is the fifth SUFD review. The COV will be chaired by **John Tranquada** and will occur on April 12 – 14, 2016.

The COV will make use of the Portfolio Analysis and Management System (PAMS) process and will examine SUFD over FY13–FY15. The COV will examine 17 facilities, construction and MIEs, and the Accelerator and Detector Research Program. The COV will consist of four panels. Five of the 14 participants are BESAC members.

Updates on the recommendations from the 2013 COV will be presented to the 2016 COV.

Discussion

None

PRESENTATION ON THE SNS PROTON POWER UPGRADE

Thom Mason, Director, Oak Ridge National Laboratory (ORNL), introduced the two projects under consideration: the Spallation Neutron Source (SNS) Proton Power Upgrade (PPU) and the SNS Second Target Station (STS). The SNS PPU is a distinct project from the SNS Second Target Station (SNS STS) but the two projects are closely linked. The science case for both is established, and R&D has set the technical foundation.

DOE and BESAC publications dating back to the 1980s developed the case for a new neutron source. By the 1990s, the value of an accelerator source had become clearer with specifications that allow for upgrades deemed desirable. In the last six years, there has been a review of a long-pulse mode. Since the BESAC facilities prioritization in 2013, the SNS facilities have been discussed with the technical community to identify needs that could be filled and technical requirements.

The PPU and STS would double the size of the facility. ORNL has collected community input, examined the feasibility of technical concepts, and determined the science drivers to be met by the technical concepts. Background work identified the need for a short-pulse, high-brightness cold source with broad dynamic range. The long-pulse option was removed as ORNL already has the High Flux Isotope Reactor (HFIR), a long-pulse resource.

The PPU will provide increased power capabilities, greater power delivery to the first target station, more neutron flux, and a platform for STS.

PRESENTATION ON THE SNS SECOND TARGET STATION

Paul Langan, Associate Laboratory Director for Neutron Sciences, Oak Ridge National Laboratory (ORNL), reviewed how the technical goals presented by **Mason** in describing the SNS PPU will be met by the SNS Second Target Station (SNS STS).

The initial SNS started in 2006 and now operates with 19 beamlines. Two more will be added, bringing SNS to its full capacity.

Langan described the value of neutron scattering as a tool of discovery and innovation. The co-location of SNS and HFIR at ORNL with its Leadership Computing Facility and Center for Nanophase Materials Sciences provides added benefit.

A strategic science plan was developed a few years ago in collaboration with the scientific community. Four subsequent workshops led to the emergence of grand challenges and scientific capabilities needed to meet these challenges. The STS will meet these challenges and address opportunities described in the "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science" report.

The projects are ready to proceed and the existing facility was built for expansion. The PPU will require seven cryomodules and high-power RF equipment. Several magnets and kickers would be upgraded. Langan described the project as low-risk.

STS will deliver a level of brightness 20 times higher than the first target station, and is optimized for high neutron peak brightness at long wavelengths.

The scientific case supporting the proposal for STS identified 22 instruments that could drive the STS. The list of instruments has been down-selected to 12 instruments; 8 would be part of the project.

The technologies that would underpin the STS have been a focus for ORNL. Research on moderators, the target, beam choppers, and neutron optics and detectors has been pursued by ORNL.

Discussion

Tranquada asked about the frequency at which the target will rotate. **Langan** explained that it rotates at a rate of less than a half hertz. It is constant and it dissipates heat.

Langan described the user community for **Rollett**. There are more than 1,300 unique users per year. There are about 3,000 visits per year, and about 50 percent are new.

Hemminger asked about the demography of users from outside the U.S. **Langan** shared that the SNS is the world-leading high brightness source so there are many outside users with a significant number from Europe.

Olvera asked about limitations on the dynamic range of the source. **Langan** shared that individual instruments can work from picoseconds to microseconds. Different optimizations are possible.

Langan clarified for **Persis Drell** that most users use more than one instrument. As an example, there is the ability to survey using inelastic instruments at SNS then go to HFIR with much higher energy resolution. **Drell** wondered about the strategy around instruments, asking if each one specialized in a specific measurement or measured many different things. **Langan** sees both as important. Some should be optimized for specific measurement and others are reconfigurable and multi-modal. There are many different neutron scattering instruments and both approaches are important. **Mason** added that the instruments are factored differently than in the x-ray world. Neutrons are expensive and the instrument has to be optimized more narrowly. There would be only 30 instruments across the two sources, so instruments need to ne reconfigurable.

Hemminger asked about the validity of a comment that without the STS, work would be ceded to the ESS. **Langan** shared that ESS have access to the same dynamic range but have compromised by having a long pulse. The STS would be sharper.

Langan clarified for **Hemminger** that cost and the footprint limit the power to 2.8 megawatts. **Mason** added that the determination of how high it could go was driven by the ability to make upgrades easily and by cost. **Langan** added that the dark time would be very short. Cryomodules could be added during regular maintenance periods. The dark time would be just a few months.

Langan told **Hemminger** that the spatial size of the proton beam on the target is five by five centimeters.

Hemminger noted that one issue around SNS is the coupling of real time data analysis and asked if it is more of a challenge for the STS. **Langan** described two aspects. One is providing users with usable data and recent efforts have improved this aspect. The other is the ability to quickly assess experiments in real time. This is very important for STS due to the complexity of the data. Additionally, there are plans that will have beamlines with multiple experimental probes. This will require more development.

Hemminger asked what is limiting output to 10 hertz. **Langan** shared that other frequencies could be used. **Mason** shared that this comes from the mass of the neutron. Ten hertz gives a long enough window to sweep out the dynamic range. The first target station operates at 60 hertz and is optimized for thermal neutrons. Going above 60 hertz loses the advantage for time of

flight measurements and approximates a continuous wave source. Going below 10 hertz would mean giving away too many neutrons.

Bare asked about what this will do annual operating costs. **Langan** shared that this is CD-1 so there is uncertainty, but costs are estimated to increase around $3 to $4M for PPU. STS will operate with double the number of beamlines, so costs will increase around $50M.

Langan clarified for **Rollett** that the duration for doing experiments such as a tomography experiment depends on the sample. One experiment can take 10 minutes.

Langan responded to **Piot's** interest in support for the upgrades and shared that the cavities would likely be purchased for the upgrades.

DISCUSSION OF THE PLANS AND PROCESS FOR ADDRESSING THE BESAC CHARGE

John Hemminger, shared plans to develop a subcommittee that would meet in April 2016 to prepare a draft report for the BESAC meeting in June 2016. A location for the subcommittee meeting is still being identified.

Leone commented that the facilities have a broad range of differences. He suggested that it would be valuable to hear historical data such as number of publications, examples of high profile publications, and other data. **Hemminger** noted that speakers would need to know informational requests in advance to optimize the time that the subcommittee is together.

Cuenya suggested that it would be helpful to hear from DOE how many upgrades would be possible and the timeline for doing upgrades. It would also be helpful to know if there will be projects going on simultaneously. **Hemminger** added that BES and SC are aware of these types of issues. It would be worthwhile for the subcommittee to hear this type of information in a closed session.

Hemminger offered that it could be useful to involve experts from host institutions that are proposing upgrades but offer them the opportunity to recuse themselves for conflicts of interest.

Public comment

None

ADJOURNMENT

Hemminger and **Kung** thanked those BESAC members who are leaving the Committee and for whom this is their last meeting.

Hemminger adjourned the meeting at 9:40 a.m. EST.

NEXT MEETING

The next meeting is to be held June 9-10, 2016.