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

PUBLIC MEETING MINUTES

July 13-14, 2017

Hilton Washington DC/Rockville Hotel & Executive Meeting Center
1750 Rockville Pike, Rockville, Maryland 20852-1699

July 13-14, 2017
DEPARTMENT OF ENERGY BASIC ENERGY SCIENCES ADVISORY COMMITTEE
SUMMARY OF MEETING

The U.S. Department of Energy (DOE) Basic Energy Sciences Advisory Committee (BESAC) convened on Thursday and Friday, July 13 – 14, 2017 at the Washington DC/Rockville Hilton Hotel and Executive Meeting Center in Rockville, Maryland. The meeting was open to the public and conducted in accordance with the requirements of the Federal Advisory Committee Act. Information about BESAC and this meeting can be found at http://science.energy.gov/bes/besac/

BESAC Members Present:
Persis Drell
Dawn Bonnell
Jingguang Chen
Cynthia Friend
Yan Gao
Bruce Kay
Despina Louca
Abbas Ourmazd
Ian Robertson
Frances Ross
Maria Santore
Esther Takeuchi
John Tranquada
Stephen Wasserman

Designated Federal Officer:
Harriett Kung, Director, Office of Basic Energy Sciences

Committee Manager:
Katie Runkles, DOE BES

BES Management Participants:
Steve Binkley, Acting Director, DOE Office of Science
Bruce Garrett, Director, BES Chemical Sciences, Geosciences and Biosciences Division
Linda Horton, Director, BES Materials Sciences and Engineering Division
James Murphy, Director, BES Scientific User Facilities Division

Thursday, July 13, 2017

BESAC Chair, Persis Drell, called the meeting to order at 9:06 a.m. Eastern Time (ET). Drell asked BESAC members to introduce themselves and opened the meeting.

NEWS FROM THE OFFICE OF SCIENCE

Steve Binkley, DOE, Acting Director Office of Science (SC) thanked Drell and BESAC members for their service. DOE priority areas are nuclear weapons, exascale computing, nuclear waste management, electric grid protection, and early-stage research and development (R&D) at the national laboratories. SC has historically focused on early stage research; therefore, the administration's priority on early stage R&D will be beneficial.

Binkley projected that implications of the FY18 President's Budget Request (PBR) on SC will not be known until fall 2017. DOE political appointments include Dan Brouillette, Deputy Secretary of Energy, and Paul Dabbar, Under Secretary for the Office of Science. Barbara

Helland has been appointed the Director for Advanced Scientific Computing and Research (ASCR).

The SC budget is reduced 17% in the FY18 PBR and BES's budget will be reduced 16.9% (– $317M). House marks have been completed and the Senate marks are anticipated at the end of July.

Discussion

Persis Drell asked about the Undersecretary for the Office of Science's role; if it will continue to be one position or return to two positions. **Binkley** explained that under the Energy Policy Act (2005, P.L. 109-58) allows for an Undersecretary for Science and a Director of the Applied Energy Programs. During the second Obama administration the applied energy programs were moved under the purview of the Undersecretary. Both positions have been announced, implying the administration will return to having two separate positions.

NEWS FROM OFFICE OF BASIC ENERGY SCIENCE (BES)

Harriett Kung, Director BES, announced six new initiatives from the President: reviving nuclear energy, financing overseas coal energy plants, developing a petroleum pipeline to Mexico, selling natural gas to South Korea, exporting natural gas from Louisiana, and creating a new offshore oil and gas leasing program.

The FY17 BES appropriation was $1.871B, an increase of $22.5M which reflects strong, positive support. Facilities are funded at or above the optimal level and Computational Chemical Sciences were funded at $13.5M. The late appropriation decisions required two spending approaches, a laboratory solicitation for up to $6M and open solicitations for university grants for the remaining $7.5M.

In FY17 BES will finish the Major Item of Equipment (MIE) project National Synchrotron Light Source II Experimental Tools (NSLS-II NEXT) at Brookhaven National Laboratory (BNL). NEXT has delivered five world-class instruments with a total project cost of $90M. CD-4 approval was recommended at the May-June Office of Project Assessment Review. The Basic Research Needs (BRN) workshop in August 2017 will focus on reviving and expanding the nuclear energy sector and a Roundtable on X-ray Free Electron Lasers (XFEL) will be held in October 2017. The BES 2017 Program Update and BRN Workshop Report Brochures have been published as part of the BES communication strategy.

The BES FY18 budget request ($1.554B) is an overlay of administration, SC, and BES priorities. A targeted decrease of activities will address the BES budget reduction of $317M. BES feels it is important to continue to advance the forefront of the discipline as reflected in the priorities, the BESAC Transformative Opportunities Report, and the BRN reports. The 36 Energy Frontier Research Centers (EFRC) will be re-competed in FY18, but the ~10% reduction affects the number that can be supported. No funds are requested for the Energy Innovation Hubs and BES will work with the Joint Center for Artificial Photosynthesis (JCAP) and the Joint Center for Energy Storage Research (JCESR) to ensure that the tools and knowledge generated in the hub are broadly disseminated. Four of the five x-ray light sources will continue operations at ~10% below FY17. Stanford Synchrotron Radiation Light Source (SSRL) at Stanford Linear Accelerator Center (SLAC) National Accelerator Laboratory will have limited operations up to the first quarter of FY18 before transitioning to warm standby status and the Spallation Neutron Source and High Flux Isotope Reactor operations will be reduced by ~15% from the FY17. Three of the five Nanoscale Science Research Centers (NSRC) will be supported at ~9% below

FY17 with reduced scientific thrusts and core capabilities. All user facilities will experience reduced hours and support, beamline and instrument shutdowns, and deferred maintenance, upgrades, and procurement activities. Linac Coherent Light Source II (LCLS-II) and Advanced Photon Source Upgrade (APS-U) construction projects will continue to be supported given the global push for XFEL. The overall appropriation for SC is $5.392B and $177M supporting program direction in the FY18 House Energy and Water Development (HEWD) Subcommittee Bill. In lieu of the two Energy Innovation Hubs, the recommendation is $10M for competitive awards, $15M for Experimental Program to Stimulate Competitive Research (EPSCoR), and funding for continued operations of all 12 BES User Facilities. The HEWD mark for BES funding is 20.39% higher than the FY18 PBR.

Kung concluded her remarks echoing the strong linkage between BES and Exascale Computing and Quantum Information Sciences (QIS). BES has a very strong linkage with QIS in the areas of quantum materials and quantum chemistry, nanoscience centers, and research beyond the current generation of qubit concepts. Finally, Kung referenced the new BESAC charge to produce a report commemorating BES program's major scientific accomplishments.

Discussion

Drell thanked Kung for the thoughtfulness put into the FY18 BES plan and asked if Kung or Binkley had any knowledge of the funding level that would be put in place should FY18 begin with a continuing resolution (CR). **Binkley** responded that the level depends on whether or not full deliberation of the House and Senate versions was conducted. Should the Congressional votes be incomplete the funding level is bounded by the lowest request, which includes the PBR.

Bruce Kay asked about the Early Career Awards (ECA) in light of the PBR. **Kung** said that ECA is considered part of core research and the emphasis on ECA will remain the same.

Abbas Ourmazd inquired if exascale computing involved only hardware (HW) or includes software (SW) and algorithms. **Kung** referred to Helland's forthcoming presentation.

Cynthia Friend asked when the EFRCs might be re-competed if there is a CR. **Kung** said BES is in discussions with senior leadership concerning when the solicitations can be issued.

Jingguang Chen asked if there will be an open competition for the Energy Hub should the $10M be included. **Kung** said the House mark language seems to indicate competitive awards.

Drell adjourned BESAC for a break at 10:15 a.m. and reconvened the meeting at 10:50 a.m.

FUTURE OF COMPUTING: PRESENTATIONS AND PANEL DISCUSSION

Barbara Helland, Advanced Scientific Computing Research (ASCR) discussed why computing is an important partnership between BES and ASCR. ASCR is starting quantum research in Scientific Discovery through Advanced Computing Institutes (SciDAC) and Research and Evaluation Prototypes. ASCR is anticipating receiving proposals for quantum applications and quantum testbeds. Exascale computing is necessary to address problems with current technology, including the end of Moore's Law and Denard Scaling, limited frequency on chips, smaller chips, and materials problems. Programming has become more difficult because of increased transistor count and finding parallelism in sequential machines with multiple cores. The highest energy expense in computing is moving data in and out which requires machine designs of the future to focus on bringing the compute to the data.

The Exascale Computing Program (ECP) focuses on application readiness in a co-design format. ECP is working with the system SW and HW vendors to understand what processors and machines will look like in 2021-2022. ECP has defined releases of data to test the applications ensuring progress is made and tools are available when they are needed. ECP is strictly R&D; the facilities will handle upgrades and are in charge of installing the machines. ASCR is looking to BES to help extend complementary metal–oxide–semiconductor (CMOS) and Silicon, and is looking forward to seeing if Silicon or Carbon Nanotubes can be used to continue CMOS. SC has held several workshops for non-CMOS options. New technologies beyond CMOS, such as neuromorphic and QIS, are also being considered. There have been two ASCR Funding Opportunity Announcements in 2017 on Research & Evaluation Prototypes, a partnership call for research in quantum algorithms, the neuromorphic Grand Challenge, and four small projects in machine learning.

Carl Williams, National Institute of Standards & Technology (NIST) discussed QIS, proposed why BES and SC should be interested in QIS, and explained NIST's engagement in QIS. QIS is the convergence of quantum materials and information science, a realization that information processing is fundamentally physical, and that quantum enables processing in a way that is different from any classical processor. QIS exploits unique quantum properties such as coherence, superposition, entanglement, and squeezing to acquire, transmit, and process information in ways that greatly exceed existing capabilities.

NIST's first workshop on quantum computing involving industry was in 2001. QIS is a revolutionary idea and companies have been monitoring it. Judging revolutionary science means looking for the first niche application. The underlying technology and the niche applications in QIS are in sensing and metrology. The future of technology is based on QIS and the ability to control these systems. QIS technology will drive economies the same way that the transistor and information science gave rise to today's economy.

The BES mission statement reads, "BES supports fundamental research to understand predict and ultimately control matter and energy …" QIS is the ultimate in control, it is part of the SC and BES's responsibility because the future of understanding, predicting, and controlling matter and energy is about being able to do it at a quantum level. QIS will lead to fundamental impacts on BES's mission. Potential applications of quantum computers include solving basic physics problems, optimizing commercially important problems, accelerating search, and performing simulations. QIS has implications for national security, economic competitiveness, and the frontiers of science. QIS is at a tipping point as the U.S. and international companies invest in it and foreign competition grows rapidly.

NIST started in QIS in part because of the atomic clock. Atomic clocks are accurate to one second to the age of the universe. Integrating atomic clocks down to 10^{17} in less than an hour requires entanglement. Entanglement will enable deep sea and deep space explorations and improvements to the Global Positioning System (GPS). C. Williams concluded stating QIS is coming and it is going to have a broad impact on basic science research, on ASCRs missions, on HEPs missions, and on BES. BES is needed because quantum materials is crucial, and in return the quantum computers will be able to simulate and help define how to build better quantum materials.

Stan Williams, Hewlett Packard, discussed computing for the new era and focused on the end of Moore's Law, noting that for nearly 40 years so much interest has been in transistors that computing has been forgotten. S. Williams explained four opportunities that exist now, memory-centric computing, high performance open fabric to democratize computing, dot product engine, and chaos as a computing resource.

Eliminating von Neumann architecture and memory-centric computing yields an almost instant three orders of magnitude improvement in computation. The general idea of changing architecture is to put all the memory in the center of computer and put the processing around the periphery. The memory-driven computing (MDC) demonstrator has been operating since October 2016. MDC has several issues: moving data using fast persistent memory in fast memory fabric (optical interconnect), uses task-specific processing and new and adapted software. MDC is available to anyone and has had an 8000x speed-up for Monte Carlo simulations.

Gen-Z is an open systems interconnect designed to provide memory semantic access to data and devices via direct-attached, switched, or fabric topologies. Gen-Z was developed to enhance existing solution architectures, and enable new solution architectures, while delivering high-bandwidth and low-latency, software efficiency, power optimizations, security, and industry agility. Gen-Z technical advantages include memory media independence, multipath, scalability, security and isolation, advanced workloads and technologies, mechanical compatibility, high-speed signaling rates, and high-efficiency protocol.

By creating hyper-optimized computing elements based on accelerators that plug into the system and are optimized for a particular problem there are potentially factors of 1M+ improvement over current computational capability. Hewlett Packard has been working on the dot-product engine which uses a memory array to accelerate vector-matrix multiplication. There is a cross bar of tunable resistors and an input of vector voltage resulting in instantaneous multiplications. The test chips have demonstrated performance improvements 1000x, and energy efficiency 100x, better than a Graphical Processing Unit (GPU).

In a computer system, chaos can reduce computational epilepsy and increase speed and performance. Hewlett Packard has built a device based on niobium dioxide (NbO_2). A large amount of time has been spent at three synchrotrons (Advanced Light Source, Stanford, and Argonne National Laboratory) to understand the materials science going on inside of these. An *in situ* and *in operando* scanning transmission x-ray microscope (STXM) has been built with the staff at these institutions. The STXM enables understanding what is occurring inside the NbO_2 devices as it operates. By applying a DC voltage to NbO_2 it can act as an oscillator or a chaotic system which replicates some of the known behavior of neurons in the brain. Hewlett Packard is also experimenting with the Hopfield network, building it in hardware, to solve non-deterministic polynomial-time hard (NP-hard) problems. The HW is being built such that it can be scaled up to experimentally look at how fast NP-hard problems can be solved. An NP-hard problem may not turn into a polynomial problem, but there will be 3-4x orders of magnitude speed up over digital.

Discussion

Drell asked Helland and C. Williams to comment on optimizing an architecture. **C. Williams** said it was a brilliant idea for looking at the quantum problem. **Helland** agreed but said ASCR has to figure out how to use those machines and how the community can benefit.

Ourmazd asked the panelists about opportunities for getting more information from better algorithms. **C. Williams** thought algorithms are not well optimized. Language structures are created to map onto the von Neumann architecture. S. Williams is suggesting a more clever way to map the language on, meaning the problem has not been considered in the right way.

Helland explained that SciDAC was started in part because ASCR realized changing algorithms could yield more speedup. With exascale and multiple cores, algorithms needed to be revisited. **S. Williams** added that there are 3x as many software (SW) engineers as HW engineers. However, nothing works without the SW layers, and SW is more difficult than HW which. There is a need for more people and more investment.

Dawn Bonnell inquired about the U.S. standing in terms of open product technologies. **C. Williams** stated that there is a lot of international competition, especially on basic research. He thought that the barrier is breaking down but there are legacies and issues yet to be resolved. **Helland** mentioned that the Top 500 list exists in the computing area. The Chinese have the first two machines on the list and the top U.S. machine, Titan, moved from third to fourth this past June 2017. The U.S. government is trying to protect the HPC vendors and infrastructure because HPC is seen as leading to economic prosperity and national security. **S. Williams** said that most companies in Gen-Z are U.S. but not all. A significant number of companies realized open systems create more opportunities and a common operating platform still provides every company opportunity to design their own chips that fit into the system. **C. Williams** added that quantum software (QSW) is largely open; to build a quantum computer requires QSW, but without a quantum computer QSW is unnecessary.

Maria Santore asked S. Williams how students should be trained in light of the ideas he expressed. **S. Williams** described two issues. First is to shift the focus from a career tied to a few companies to a career with more freedom. Second is the physical basis of computation; that physics is critically important to understanding computation. Other outstanding issues include understanding the Mott insulator, and that the end of Moore's Law is creating many opportunities to come up with a new idea and do something about it very quickly. **C. Williams** suggested training that leads to cross-, multi- disciplinary aspects and the use of teams. **Helland** agreed with C. Williams, that students need to be trained to be flexible and willing to talk to others in different fields.

Ian Robertson asked about data transfer challenges in big facilities. **Helland** stated the network is static, but it will have to become dynamic to accommodate the data influx and meet the needs of researchers. One solution was developed in partnership with SLAC and the National Energy Research Scientific Computing Center (NERSC). A burst-buffer was placed close to the processor and a FAST-port was developed to bring data in directly from SLAC to NERSC. Make this solution work on a broader scale and over long distances in real-time is a challenge. Another challenge is how the queuing structure is melded with data input and response in near real-time.

Yan Gao commented that SW, developed by users, is not always open. Also, the SW development does not properly match up with the HW development. Gao complimented Center for Advanced Mathematics for Energy Research (CAMERA) and hoped to see more facilities that bridge the gap between ASCR and BES User Facilities. **Helland** stated that ASCR supports the work done on CAMERA and with the Advanced Light Source (ALS) because it has opened the door to more possibilities.

C. Williams asked Helland and S. Williams how the environment can be changed to no longer require a verified underlying algorithm. **Helland** stated that ASCR is starting to look at algorithms that do machine learning as well as uncertainty quantification. **S. Williams** said to change the environment DOE has to be a market maker. Programs such as CORAL and PathForward are critically important because they help make a market. DOE is working to create a market to expand HPC, make it interesting for many other users, and therefore make it interesting to suppliers.

Esther Takeuchi commented that a computational chemistry colleague claimed his work, as well as high speed computing, was enabled by the demand of video intensive games. **S. Williams** stated that was an example of adapting the Graphics Processing Unit (GPU) to doing vector matrix multiplication.

Frances Ross asked how quantum computing is addressing the power demand for future large scale computing. **S. Williams** said the demand for computing is rising exponentially, but the amount of power available is fixed by the grid. He projected that there will never be a point in time where the power problem is solved. **C. Williams** said quantum computers may enable a larger amount of computation for a given power budget, but will still use power. Learning how to transduce signals by coupling multiple quantum computers is going to revolutionize things. There are tricks to be learned on the communication and computing side that will change some of the paradigms, but in the end quantum computing will use energy.

Ourmazd asked how to refocus the community to relinquish constraining the system and using new algorithms that give the system control. **S. Williams** said that for most of the world's computation the change has arrived. The challenge is to get the change into the HPC industry where something has to be perfectly verified. **Helland** added that machine learning will be a game changer; algorithms will have to change in order to figure out how to use machine learning and be effective. Adaptive SW is being built that reflects the change.

Drell asked how BES should formulate its strategy for the next few years given its potential roles for synthesis fabrication and characterization, theory modeling, and testing. **Helland** thought the strategy had been started, that the strategy is working across SC and staying informed about what is happening. **C. Williams** stated that Helland's comments reflect the multidisciplinary aspect of training students. BES needs a broad portfolio and to ensure the right investment is made at the right time and the right amount. **S. Williams** recommended that BES make computational science a formal part of the program. Computational science is appropriate to be within DOE and BES because of the potential gains to be made in energy efficiency in computing.

Drell adjourned BESAC for lunch at 12:26 p.m. and reconvened the meeting at 1:37 p.m.

BASIC RESEARCH NEEDS FOR NEXT-GENERATION ELECTRICAL ENERGY STORAGE WORKSHOP UPDATE

Esther Takeuchi, Stony Brook University, explained that the BRN workshop assessed the current status, identified high priority gaps and opportunities, and defined new insights and innovations in electrical energy storage. The workshop was held in March 2017 with 175 attendees and a deliberate selection of speakers. Six panels discussed challenges, tools and techniques, and emerging architectures of electrochemical energy storage. Each panel was asked to identify two or three themes for critical areas. Those critical themes were grouped and discussed to create five priority research directions (PRD). The five PRDs were holistic designs and multifunctional materials, capture phenomena, control and exploit, innovative assemblies, and self-healing.

Discussion

Chen asked how 175 scientists were handled. **Takeuchi** said that the number included observers and there were ~100 active participants. The committee used a deliberate and thoughtful process to choose the panel leaders. The group worked together extremely well, all participants understood the importance and criticality of the task.

Friend asked if Takeuchi thought it was a good idea to consider the PRDs in a more integrated approach with other BRN reports. **Takeuchi** said yes, that some overlap between the five PRDs was noticed. If there was no overlap among the BRN reports she would be concerned.

Ourmazd asked about input from industry. **Takeuchi** said industry participants provided alternative perspectives on the effect of different options and changes. Use-inspired science requires the perspective of the user and the implementer and then needs to be translated into fundamental science questions.

Drell asked how the PRDs would have differed five years ago. **Takeuchi** said the distinguishing elements today are the scientific capabilities such as characterization, computational methods, theory methods, and integrating those with synthesis, material design, and operando characterization. Five years ago, the vision of the BRN might have been narrower because the capabilities did not exist.

BASIC RESEARCH NEEDS FOR CATALYSIS-SCIENCE TO TRANSFORM ENERGY TECHNOLOGIES

Carl Koval, University of Colorado, presented the BRN workshop in catalysis science. The 175 attendees at the workshop in May 2017 had a goal of bringing together PRDs that would allow a more holistic view of catalysis to improve and enable new energy technologies. Three panels discussed diversified energy feedstocks and carriers, novel approaches to energy transformations, and advanced chemical conversion approaches, and a fourth cross-cutting panel, discussed capabilities and challenges in synthesis, characterization, theory and computation. New tools in precision synthesis and operando characterization and new advances in theory and computation were seen as enablers of all the PRDs. The PRDs from the workshop included constructing catalyst architectures, controlling the dynamic evolution of catalysts, deciphering complex reaction networks, designing electrocatalyst systems, and integrating data science with catalysis science.

Discussion

Gao inquired if the user facilities were asked to develop a particular kind of characterization tool to meet the needs in *in situ* and *in operando* characterization. **Koval** stated the synergy could be great, those doing the characterization could introduce new questions and the ability to solve problems could inspire the expansion, or new directions, for the capabilities. **Takeuchi** suggested engaging the user facilities by making contact in advance, explaining the challenge, and asking for input.

X-RAY FREE ELECTRON LASERS

Claudio Pellegrini, Stanford University, provided a brief introduction to X-ray lasers and XFELs, the physics and status of XFELs, the science at LCLS, and future developments. The first infrared laser was developed in 1960 and interest in X-ray lasers started in the 1970’s. Scientists at Lawrence Livermore National Laboratory (LLNL) proposed to use a nuclear weapon to drive an X-ray laser in 1980. During the Cold War, experiments with pumping cylindrical plasmas, in some cases confining plasma with magnetic fields, led to X-ray lasing around 18 nm with gain of ~100 in 1985. Lasing has been demonstrated, with limited peak power and tunability, at several wavelengths in the soft X-ray region.

A proposal in 1992, by Pellegrini, to build an X-ray FEL using 1 km of the Large Hadron Collider (LAC) Linac, producing a 15GeV high brightness beam, lead to the design and construction of LCLS at SLAC. In 2009 LCLS successfully started to work with characteristics similar or better than originally proposed. The development of XFEL's continues to grow rapidly. Beyond LCLS in 2009, there have been the Free-Electron Laser in Hamburg (FLASH) and the Free Electron laser Radiation for Multidisciplinary Investigations (FERMI) in Italy in 2010, followed by SPring-8 Ångstrom Compact free electron LAser (SACLA) in Japan in 2011, and in 2017 new lasers are being developed in China, Dalian's vacuum UV free-electron laser (VUV FEL), and in Korea, Pohang Accelerator Laboratory XFEL.

The main XFEL characteristics are a photon energy range of 10–0.1nm, peak power between 1–50 GW, line width between 10^{-3}–10^{-4}, pulse length of a few–100 fs, repetition rate between 102–106 Hz, high flexibility, and two colors with delay variable from few to 100 fs, or ns. Comparing XFEL characteristics today with those of tomorrow; wavelength and transverse coherence are the same, line width today is 10^{-3}–10^{-4}, tomorrow it will be 10^{-2}–10^{-6}, peak intensity is 2–4mJ and will be 2–100mJ, pulse duration is currently 100–4fs and will be 100–0.3fs tomorrow, and peak power is now 0.02–0.05 TW and will be 1–10+ TW.

Discussion

Ourmazd thanked Pellegrini for acknowledging the leadership of DOE in funding XFEL work and expressed gratitude to him for his leadership in the development of XFEL. There is demonstrated evidence in optical, visible lasers, and recently confirmed in XFEL, that the spikey pulses determine the time resolution, in which case one can extract very high time resolution even into the attosecond regime without any development and then algorithmically recover the very fast processes. **Pellegrini** said it is a similar resolution and there are a lot of possibilities. This is a flexible system.

Friend asked for examples of what is on the horizon that will truly make use of these facilities. **Pellegrini** stated that improvements could be made in resolution increase, controlling the special properties, charge separation, self-seeding, and terawatt XFEL optimization.

Drell adjourned BESAC for a break at 3:16 p.m. and reconvened the meeting at 3:46 p.m.

INTRODUCTION OF NEW BESAC CHARGE

Drell read the new BESAC charge, to create a report that commemorates the founding of the BES program four decades ago. Mark Kastner (BESAC member) will chair the Subcommittee. The final document is not a summary of past reports; rather it is a higher-level, shorter document. Not all laboratories, divisions, etc. will get mentioned in the report. Drell imagined a visually appealing document that is accessible to readers and tells a compelling tale of how BES activities have led to societal progress. The target groups for the report are Congressional staffers and the educated public.

Discussion

Gao requested clarification on the definition of impact and how it is measured. **Drell** stated the definition depends on the audience. While impact could be economic or societal, all impacts should be tied to the DOE mission. **Kung** added that different fields define impacts differently and the subcommittee will be composed of people with a broader view. Kung believed the breadth and depth of well-chosen examples, rather than a laundry list of accomplishments, would showcase the impact on science.

Ourmazd remarked that the Subcommittee should first determine and propose the impact criteria. **Drell** said that she and Kastner discussed completing a small survey of potential report recipients to determine their definitions of impact.

Robertson suggested the subcommittee ask for achievements attributable to DOE support, and ask funding recipients for their definition of impact. BES played tremendous role in instrumentation capabilities as well as bringing computational experimentalist together. **Drell** agreed that input from the scientific community is important. The Subcommittee will want to think about various areas; the community will have to identify a lot of targets and write many stories; the most compelling of which will rise to the top.

Bonnell thought the BESAC charge offered an outstanding opportunity to make the case for basic science, something the nation needs to hear about in different spheres. She encouraged finding new examples, those that are 20 years old, which may compelling and more impactful to the lay audience.

Kay suggested comparing and contrasting two synergistic areas, the development of enabling scientific tools and scientific discovery on its own to show how the enabling tools facilitate scientific discovery. **Drell** referred to George Crabtree's talk at the February 2017 BESAC meeting. Crabtree conveyed that there are a lot of disparate pieces whose direction is unknown, and then an initiating event brings different things together creating a dramatic new technology, such as the iPhone. She said it is not an easy story to tell; while the community feels it, it has not always been communicated.

Steve Wasserman referred to the BBC series, Connections, which showed technology's development through history, illustrating that different branches feed onto the same trunk to tell a whole story. The pharmaceutical industry routinely experiences this because different drugs have multiple uses.

Chen asked about the subcommittee's knowledge of the balance between facility development and individual scientific discovery over the last 40 years. Chen suggested seeking input from BES funded principal investigators (PI). **Drell** said Kastner agreed to chair the Subcommittee on the condition of access to program managers who have a broad view of the portfolio. Drell reiterated that what is important is not the specific discoveries but the story.

Friend commented that it is important to humanize science, to bring people into the picture, to make it really cool to be a theoretical physicist, for example. **Drell** added that the subcommittee will have a communications professional supporting their work from Day 1.

Ross recommended a multimedia aspect be added to the report. **Drell** agreed that multimedia would be good and that there is a steady gradient that correlates with age. **Kung** said multimedia could be considered, but ultimately a report was requested.

Ourmazd suggested consulting with professionals who convey messages such as the Alan Alda Organization and that the process should be put before BESAC, in consultation with Kung, for input. **Drell** indicated she would look for volunteers and that Kastner had requested a smaller group size, between 12-15 members.

Despina Louca asked if such a report was typically requested and the reason for the charge. **Drell** said the 40th year anniversary was the triggering event. Such a report is not something requested on a regular cycle. **Kung** said this is the first time such a report has been requested.

Kay asked about the composition of the subcommittee. **Drell** said more than half of the subcommittee should be BESAC, but external membership is also acceptable.

Friend suggested the report begin with a description of DOE. **Kay** added that the report should also explain where BES fits within DOE. **Drell** asked if BESAC members recalled a report that captured their attention.

Ourmazd encouraged the Chair to ensure that the right people volunteer. **Drell** assured BESAC she will assist Kastner to create a diverse group. **Ourmazd** asked if there will be a regular report from the subcommittee to BESAC to seek guidance. **Drell** anticipated a report at the winter 2017 BESAC meeting and a near complete report by summer 2018. **Ourmazd** explained that he thought the terms of reference the subcommittee sets for itself are important to discuss with BESAC before doing a lot of work. **Drell** rephrased saying sharing early and often with a variety of stakeholders is a good way to get the best outcome.

Ross commented that the Materials Research Society (MRS) arranged Congressional visits to explain the importance of materials science. MRS has a lot of information on discoveries that have had an impact. Ross mentioned that 360^o videos of what goes on inside science laboratories is appealing. She hoped that the report would not require a lot of reinvention of material. **Drell** pled with BESAC to provide or point the subcommittee to good stories and material. In her opinion, the most common challenge to such materials is density; pairing down is essential. There are times when less is more and this will be one of those times.

Takeuchi asked if workforce readiness, the role of young investigators, constituted an impact. **Drell** said she could imagine it would be compelling and could imagine workforce readiness would not be compelling. Drell suggested Takeuchi develop the idea into a story thread; she thought a lot of the stories will weave different topics together.

Bonnell stated that some stories from laboratories became part of the June 2017 report from Advanced Scientific Computing Advisory Committee (ASCAC), *Independent review of Laboratory Directed Research and Development (LDRD) work of the DOE Laboratories (Labs).* **Drell** asked Bonnell to point the subcommittee to those stories.

Louca stated that the 40 year retrospective will be challenging and she hoped the subcommittee would have resources beyond program managers; people with knowledge of what has been going on in the last 40 years to make it profound.

Santore suggested the subcommittee begin with what would impress the target audience and work backwards to the discoveries. **Wasserman** referred to Felice Frankel, a photographer at Harvard, saying the story needs to look spectacular, to use images.

Drell closed the discussion telling BESAC members to expect an email from the BESAC Chair to solicit volunteers. Drell said she will encourage Kastner to provide regular communications to BESAC.

Public Comment Session

None.

Drell adjourned the meeting for the day at 4:25 p.m.

Friday, July 14, 2017

Cynthia Friend was the Designated Chair for the second day of the BESAC meeting.

CHEMICAL SCIENCES, GEOSCIENCES AND BIOSCIENCES (CSGB) DIVISION COMMITTEE OF VISITORS (COV) REPORT

Bruce Kay, Pacific Northwest National Laboratory (PNNL), reviewed the COV report for the CSGB division, whose meeting was held in March 2017. There were three panels mapped onto the divisions of CSGB. This COV was the first of 20 that utilized the Portfolio Analysis and Management System (PAMS) system to access and examine only electronic materials. The COV report contains four major findings, three major recommendations, and four other suggestions. The major findings were program managers were dedicated, focused, professional, committed, and effective; the portfolio includes a balance of international scientists at all career levels; the practice of encouraging submission of white papers is effective; and navigating PAMS proved to be more challenging than anticipated. The three recommendations were opportunities and resources for program officers to travel to national and international conferences, modules and improvements to the PAMS system, and broaden the scope of strategic planning. Other suggestions included: provide funding decision information to the PI in writing as well as over the phone; hold occasional cross-team PI meetings; create uniformity in the structure and content of program stature documents; and add an explanation checkbox system to the white paper email responses.

Discussion

Chen asked Kay to expand on recommendation 3 in terms of synergy. **Kay** indicated recommendation 3 referred barriers breaking down when teams talked to each other or areas held discussions.

Tranquada asked about advantages and disadvantages of holding the COV off site, away from the DOE building. **Kay** thought there were many advantages but did not see any disadvantages.

Ourmazd asked if the panel considered the contribution of the annual contractors meetings. **Kay** said team leaders from various programs often invite people from other programs those meetings. Contractor meetings were working smoothly thus the COV did not make comments.

Friend called for a motion to accept the COV report, **Ourmazd** moved to accept the COV report and **Robertson** and **Bonnell** seconded the motion. BESAC members unanimously agreed to accept to CSGB COV report.

DRUG DISCOVERY AT BES X-RAY LIGHT SOURCES

Steve Wasserman, Eli Lilly & Company, explained the use of BES X-ray Light Sources in relation to drug development. Drug discovery is a major research operation totaling $69.4B in 2016 in the U.S. Only 1 in 10,000 drugs make it to market and it costs ~$2.6B and takes 13 years of development to get a drug to market. Drug discovery and development would not be possible without the innovations and equipment at DOE facilities, both in how to make protein targets and how to study them at the synchrotron. Historically, the first inhibitor bound to a protein was in 1964, the first synchrotron diffraction was in 1976 with an exposure time of 5 hours. What took 5 hours in 1976 is now done in 15 seconds at the NSLS-II.

The synchrotron allows tuning of the x-ray to the absorption edge of a particular element located in the protein. When Eli Lilly started using the synchrotron, the tunability of the source was important. Analysis methods have improved to the point that the brightness and the intensity have come to the fore again. The pharmaceutical industry made a commitment to get involved at the beamlines. Pharmaceutical work is primarily done at the APS: Industrial Macromolecular Crystallography Association, ALS: Berkeley Center for Structural Biology, Beamline 5.0, and APS: Lilly Research Laboratories.

The synchrotron is only a small part of developing a protein structure. Crystallization time is greatly reduced because the intensity at the synchrotron allows the use of smaller crystals. The volume of crystals that can be sent to the synchrotron is 1,000 times smaller than what would be needed for a home x-ray source, and the data rate is extremely high compared to the home x-ray (home x-ray = 2-3 crystals per day, synchrotron = 30-40 crystals per hour). The synchrotron also gives much better data quality meaning automatic data analysis can happen much more readily.

Academic assignments at the synchrotron are 7x that of industry. The impact of the synchrotron on pharmaceutical research is underestimated because of the high volume of work completed per hour compared to typical academic colleagues. In terms of data sets and useful electron density maps, the pharmaceutical yield is ~1 order of magnitude higher in terms of how many data sets lead to protein structures or at least electron density maps that can be evaluated. In October 2016, Eli Lilly and SGX crossed its 10,000th protein structure. As a comparison, on the day Eli Lilly crossed 10,000 the Public Data Bank had 123K protein structures. As one company, Eli Lilly has generated 8% of the total world-wide protein structures.

Discussion

Louca asked if incorporating synchrotron radiation reduced the time it takes to develop a protein structure. **Wasserman** said because current problems are harder, the synchrotron has helped keep the process time from expanding.

Ourmazd asked Wasserman to elaborate on the possible use of XFEL. **Wasserman** said that there have not been any XFEL protein structures yet. Eli Lilly will experiment with XFEL, but the focus is protein co-crystal structure with a ligand and it would have to be one Eli Lilly is willing to release publicly, it is very difficult to do in a proprietary mode.

Takeuchi asked if Eli Lilly could provide stories about the impact of the synchrotron and diffraction over the past 40 years. **Wasserman** said he believed they could, for example Eli Lilly revealed a structure-based project as part of their support for BES budget and the APS-U during the Congressional budget hearings in June. Eli Lilly revealed, for the first time, one of its structure-based projects, which is about to be filed with the FDA for approval. There are other examples; the APS has used Kaletra, an HIV treatment, the protease work on Hepatitis C (Hep-C) and the combination therapies that work for Hep-C.

Bonnell asked for his perspective on the evolution of pharmaceutical partnerships with the national laboratories. **Wasserman** said partnership models are changing; diseases are too hard and complex and is not economically feasible to continue working alone. Methods development and specific proprietary targets and drugs are areas of cooperation at Eli Lilly.

Ross asked about the importance of cryo-electron microscopy (cryo-EM) compared to the x-ray. **Wasserman** responded that cryo-EM investigation at Eli Lilly is done externally. Presently, cryo-EM cannot approach the same throughput as x-ray work. If a crystal can be grown, the synchrotron is the first choice. Crystallization challenges are known in such things as multi-protein complexes. For example, the nuclear pore complex has 16 individual proteins that all associate and the crystallization is difficult. The structures of those 16 proteins individually can be determined by other means and then the cryo-EM data can be used to assemble what is seen from the electron microscope into the structure of the whole complex using the individual pieces of the puzzle.

BES AND THE NATIONAL LABORATORIES, ADVANCING DOE MISSIONS FOR 40 YEARS

Steve Ashby, PNNL, provided an overview of BES, DOE, and the National Laboratories over the past 40 years. The current form of DOE and BES were founded in 1977. The foundational goals of BES in 1977 were to explore fundamental phenomena, create scientific knowledge, and provide unique user facilities necessary for conducting basic research. In 2016, 150 entities, 17 national laboratories, and 47 states and the District of Columbia were associated with BES. Across the 12 user facilities there were 15,000 users, 5,400 investigators, and 1,700 students, all working in 25 research areas on more than 1,000 individual projects, and producing more than 3,500 publications. BES has had 9 Nobel prizes since 1986 in Chemistry and Physics.

Collectively the national laboratories (labs) receive $14B in annual funding, employ 57K staff members, produce 11K publications, and hold 5.8K active licenses. The national labs exist to support the nation and in particular to advance DOE missions across all four of the mission areas. The national labs deliver impact by addressing national needs, stewarding science and technology capabilities, enhancing economic competitiveness, and operating unique facilities and instrumentation. The labs respond to crises such as terrorist attacks, oil spills, nuclear disasters, and gas leaks. The national labs operate the facilities for the benefit of the community, and offer the nation a system of laboratories.

Over time the labs along with DOE have developed a mature and best in class construction and project management capability. The government has been able to turn to the captive workforce of expertise at the national laboratories and ask for honest technical advice on how to address challenging problems. There are 12 user facilities organized in three categories, x-ray light sources, nanoscale, and neutron scattering. The labs are part of the BES family in terms of hosting the user facility as well as performing research. Of the 36 EFRCs, nine are led by national labs, and all involve partnerships with academia and industry.

The 1977 goal of energy independence is largely being achieved. Fracturing technology and the natural gas revolution have been key parts of that success. Natural gas has changed the energy landscape for the world, the U.S., and the economy. Ashby stated that the oil industry will rightfully take credit for the invention and exploitation of horizontal drilling technology. The national labs can rightfully take credit for the fundamental science that went into the characterization, imaging, and understanding of the subsurface and the geosciences that allowed horizontal drilling technology to be exploited to the benefit of the energy revolution today.

The labs help BES envision the future. SC and BES have honed a time-honored process for looking at the future which is inclusive in terms of science for discovery, national needs, and the future of user facilities. SC and BES do that through the BRN workshops which the labs often host, help organize, and assist with the hard follow-on work of translating a workshop report into programs.

Delivering an exascale platform in the next few years will showcase the emergence of support the national labs can offer in terms of leadership-class computing. Exascale will enable new discoveries in areas of relevance to BES, such as in quantum materials and chemistry, catalysis, and photosynthesis and light harvesting. In addition to looking at how to exploit exascale computing for scientific advances, the community needs to consider what is beyond exascale. Beyond exascale leads to thinking beyond CMOS, which further ventures into interesting materials, quantum computing, and DNA-based computing, for example. BES is not only benefitting from exascale simulation and being a driver for it, but contributing to what is going to be beyond exascale in terms of QIS.

Discussion

Gao asked Ashby to comment on partnerships with industry, especially at user facilities. **Ashby** believed that a large number of industries have benefitted from partnerships with the laboratories and DOE, including the use of the user facilities. For example, PNNL partners with General Electric (GE) in the grid area; the computer industry has a decades-long use of the light sources to test chips; and the automotive industry also utilizes user facilities. There will be an increasing number of partnerships between the national laboratories and industry. The labs are trying to get fundamental discoveries to industry for commercialization. However, there is a philosophical debate occurring about the role of government in helping to make the transition from laboratory to industry. The Secretary of Energy has asked the national laboratories for their input on this debate. A number of examples have been collected that show the impact the national laboratories have had in partnering with industry. However, the labs can do a much better job articulating those successes and it will be interesting to define the role, under the current administration, of that engagement.

Chen requested clarification on the number, 150 academic and industry institutions, listed. He asked if that number only represented institutions that receive BES grants. **Kung** confirmed that the 150 were the performers not the users.

BESAC CHARGE DISCUSSION

Friend opened the floor for further discussion of the BESAC charge.

Chen thought a BES or BESAC person should follow up to get more concrete examples from Wasserman and Ashby. **Friend** agreed and said there is a good start on the charge and to bear in mind some of the comments about humanizing science and making the stories exciting and visual.

Public Comment Session

None.

Friend adjourned the July BESAC meeting at 10:30 a.m.