

MINUTES
Biological and Environmental Research Advisory Committee
October 1–2, 2014
Rockville Hilton Hotel and Conference Center
Rockville, Maryland

BERAC Members Present

Gary Stacey, Chair	G. Philip Robertson (Wednesday only)
Dennis Baldocchi	Martha Schlicher (Wednesday only)
Janet Braam	Jacqueline Shanks
James Ehleringer	Gus Shaver
Susan Hubbard	David Stahl
Anthony Janetos	Judy Wall
Andrzej Joachimiak	John Weyant
L. Ruby Leung	Minghua Zhang (Wednesday only)
Sabeeha Merchant	Huimin Zhao
Karin Remington	

BERAC Members Absent

James Hack	William Schlesinger
Judith Curry	Warren Washington

About 50 others were in attendance during the course of the two-day meeting.

Wednesday, October 1, 2014
Morning Session

The meeting was called to order at 8:59 a.m. by the chairman, **Gary Stacey**. He asked each Committee member to introduce himself or herself and to relate what was going on in his or her professional life. Stacey noted that Warren Washington, Gus Shaver, and Judith Curry are rotating off the Committee and that their input was highly appreciated. David Thomason has announced his retirement from DOE after 16 years as the Designated Federal Officer of BERAC, effective in January 2015.

Patricia Dehmer was asked to present the news from the Office of Science (SC).

DOE is awaiting confirmation of its nominees for Director of SC and Undersecretary for Science. Elizabeth Sherwood-Randall was confirmed as the Deputy Secretary of Energy. Michael Knotek, the Acting Deputy Under Secretary for Science and Energy, has staffed the office with very competent people. That office is looking at protocols and best practices of the different offices within SC.

Marks on the 2015 budget have been mixed. Those for the offices of High Energy Physics and Nuclear Physics have been above the President's Request. The marks for Basic Energy Sciences were at the President's Request in the Senate and below the President's Request in the House of Representatives. Those for the Office of Biological and Environmental Research (BER) were very different in the House and Senate but were offsetting.

Briefings are being provided to the Office of Management and Budget (OMB) for the 2016 President's Request.

The Secretary of Energy Advisory Board (SEAB) will be looking at the national laboratories. Another assessment of the national laboratories is in process under a congressional mandate. The latter committee is looking at DOE's strategic plan and how it translates into work at the national laboratories. The SEAB Subcommittee, a standing subcommittee, has taskforces looking at general contracting; work for others; technology transfer; laboratory-directed R&D; and the roles and responsibilities of Headquarters,

laboratory management, the site offices, etc. These committees will be important and will be taken very seriously.

Workforce development is a small but important part of the DOE budget. In 2013, OMB directed cuts to science, technology, engineering, and mathematics (STEM) education and workforce training programs in more than 10 Federal agencies. More than 115 programs were terminated, including the following DOE programs:

- Computational Sciences Graduate Fellowship
- Summer School in Nuclear Chemistry and Radiochemistry
- Global Change Education Program
- QuarkNet [Office of High-Energy Physics (HEP)]
- National Undergraduate Fellowship Program in Plasma Physics and Fusion Energy Sciences
- Plasma/Fusion Science Educator Programs
- Graduate Automotive Technology Education
- Wind for Schools
- Nuclear Scholarships/Integrated University Partnerships

A primary motivation for OMB's decisions was to eliminate small programs in favor of aggregating them into larger programs at fewer lead agencies, notably the National Science Foundation (NSF). This came as a real shock to the agencies, many of which have programs to attract young people to mission work and laboratories. Congress was not happy with these terminations and provided one-time support for the programs in FY14. OMB has now softened its position slightly and will consider funding programs that are justified by the agencies and their offices.

Each of SC's 6 federal advisory committees, 7 SC associate directors, and 10 SC laboratory directors were asked for their expert assessment on the following:

- Which STEM disciplines are not well represented in academic curricula?;
- Which STEM disciplines are in high demand, nationally and/or internationally, resulting in difficulties in recruitment and retention at U.S. universities and at DOE laboratories?;
- Which STEM disciplines for which the DOE laboratories may play a role in providing needed workforce development?; and
- What recommendations for programs at the graduate student or postdoc levels can address discipline-specific workforce-development needs?

The responses were to be the "evidence" to be provided to OMB.

Responses were received from everyone who was polled. The input identified both program-specific workforce-development needs and cross-cutting workforce-development needs. More than 50 SC program-specific disciplines were recognized as needing greater emphasis for workforce training. There were four cross-cutting areas identified:

- Computational sciences
- Accelerator and detector R&D
- Instrumentation
- Nuclear chemistry/radiochemistry

Interdisciplinary sciences were emphasized by several programs and national laboratories, particularly by BER and one laboratory director.

The single most-cited program was the Computational Sciences Graduate Fellowship. It is SC's highest priority of the programs to be restored. The Secretary was briefed and told that this was the most important, longest-lasting, and most studied workforce-development program in DOE. It has great impact and is conducted with great rigor.

All responses identified programs, such as graduate fellowships, research practicums at national laboratories, thesis-part research conducted at national laboratories, laboratory-based postdoctoral appointments, topic-specific workshops or "summer schools," and outreach activities.

One comment from a respondent read, “The demand for graduates in computational sciences and engineering far exceeds the supply from academic institutions. ... There is a large industry demand for students with master’s level education, which drains the number of students pursuing advanced degrees.”

Tabulations of the BERAC, BER, and national-laboratory inputs analyzing BER’s workforce-development efforts show the different topical areas and where the recommendations came from. Capital analysis was conducted, and the data are now being drilled down into.

From the FY15 interactions with OMB about STEM, passback from OMB supported the Administration’s STEM-education consolidation strategy, and provided no funds for activities consolidated in FY14. However, OMB recognized that DOE has mission-specific workforce needs in STEM fields and that the national laboratories are a unique resource for training workers in STEM research and development. OMB requested that STEM workforce-development activities in SC include an evidence-based statement of the workforce need; a clear statement of program goals; documented best practices that will be followed to ensure a diverse applicant pool and an unbiased selection procedure; and a mechanism for tracking program outcomes and evaluating success.

The Computer Science Graduate Research Fellowship (CSGRF) has all of these, but most of the other workforce development activities in SC do not. The level of rigor in those other programs must be increased and documented for OMB in terms of best practices etc. Serious consequences could occur if there is not this improvement in the workforce-development programs.

DISCUSSION:

Wall asked if there were metrics. Dehmer replied, yes.

Zhang asked if programs would be terminated if they have not documented their activities. Dehmer replied that they must have goals, metrics of performance, and assessment of progress toward goals. About 30 activities were terminated right off the bat when she took over as Acting Director.

Joachimiak noted that many people have gotten important training at the national laboratories, especially science, technology, engineering, and mathematics (STEM) students. He expressed his hope that these opportunities continued. Dehmer answered that software has been developed for tracking participants in such programs, and funding for such programs has been increased.

Shanks asked what the right metrics were and where the Department was going in this process. Dehmer replied that the Department currently does not know what to do with the tracking data and is going to have protocols developed for such analyses.

Stacey asked if there were any reason to be optimistic about funding for university research. Dehmer said that she thought that there was. A few years ago, when it did not look like things could get any worse, along came the Recovery Act. She said that she was not discouraged and urged researchers to be ready for a rebound.

Merchant noted that the only time universities have vigorous tracking is in federally funded programs. That tracking and its analysis are very important. They have made contributions to coursework development and other components of academic programs. Dehmer thanked her for that comment.

Sharlene Weatherwax was asked to give an update on the activities of BER.

Under the new reorganization, BER operates within SC, which reports to the Under Secretary for Science and Energy, who reports to the Secretary of Energy.

FY14 has been officially closed out. The hard work of the program managers was acknowledged. This meeting falls at the beginning of FY15. Funding for the Biological Systems Science Division (BSSD) for that fiscal year is \$299.89 million in the President’s Request, \$290.49 million in the House mark, and \$299.89 million in the Senate mark. Funding for the Climate and Environmental Sciences Division (CESD) is \$328.11 million in the President’s Request, \$249.51 million in the House mark, and \$327.64 million in the Senate mark. The total BER funding is \$628 million in the President’s Request, \$540 million in the House mark, and \$627.5 million in the Senate mark. Congress did not enact a budget; rather, they passed a continuing resolution that lasts until December 11, 2014. Under the continuing resolution, BER has been allocated \$120.23 million until December 11.

The House had strong support for biological programs but significantly decreased funding for BER climate programs. The Office is planning its funding on the basis of the lower mark in case it is held to that level of funding. There was a similar period of uncertainty in FY14, but the community met all its goals as measured by the appropriation metrics.

BER currently has a number of vacancies. Wanda Ferrell and John Houghton have retired, and Jay Fitzgerald (AAAS Fellow) will be working in another DOE office. A new atmospheric research program manager, Shaima Nasiri, has been hired in CESD.

Weatherwax congratulated a large number of BERAC members and BER principal investigators (PIs) for their achievements, recognitions, and awards. She also congratulated the national laboratory R&D 100 Award winners; the national laboratories won 31 of 100 awards in 2014 with three of them related to BER.

There are new requirements on digital data that resulted from a presidential order based on the Administration's goals for getting technical information out to the public. DOE has developed and rolled out its Public Access Gateway for Energy and Science (PAGES), a web-based portal that will provide free public access to accepted peer-reviewed manuscripts or published scientific journal articles within 12 months of publication.

All proposals for research funding submitted to SC are now required to include a data-management plan (DMP) that describes whether and how the digital research data produced during the course of the proposed research will be shared and preserved. SC has a data-management website to guide proposers. A DMP should

- Describe whether and how the data will be shared and preserved; at a minimum, DMPs must describe how data sharing and preservation will enable validation of results or how results could be validated if data were not shared or preserved
- Provide a plan for making all research data displayed in publications open, machine-readable, and digitally accessible to the public at the time of publication
- Consult and reference available information about data-management resources to be used in the course of the proposed research
- Protect confidentiality; personal privacy; personally identifiable information; and U.S. national, homeland, and economic security
- Recognize proprietary interests, business-confidential information, and intellectual property rights, avoiding significant negative impact on innovation, and U.S. competitiveness

A new BERAC charge requests that the Committee recommend the major next initiatives for field-based research that capture a multidisciplinary approach and build on observations and modeling. Those recommendations should

- Identify candidate geographic regions that are poorly understood with respect to Earth-system predictability
- Identify major cross-cutting gaps in BER sciences that limit the understanding of the predictability of Earth science across numerous geographic regions
- Exploit unique BER assets
- Exploit science capabilities of both CESD and BSSD
- Provide opportunities for collaborations involving other federal or international agencies
- Exploit emerging scientific discoveries and advanced technologies from other disciplines

DISCUSSION

Zhang asked how long data should be preserved. Weatherwax replied that that topic is discussed in the FAQs. The standard best practice is to contribute the data to a community facility.

Wall asked when one should remove obsolete data. Weatherwax answered that the procedures do not mention duration. There is no requirement to delete data. Sometimes, a re-analysis of "old" data turns up something very important.

Merchant noted that there are lots of types of data. Some researchers have access to institutional deposition sites. But there are data that might not fit into such databases. Self storage is not sustainable;

researchers retire and die. Weatherwax responded that one should state one's best attempts and see how the reviewers assessed that approach. Merchant replied that DOE should consider the appropriate methods for retention of data and the associated costs. One sees a lot in the press about non-reproducibility. But with DOE data, large facilities are needed to produce *and reproduce* the data, so minutia are not reported. The types of data to be preserved should be looked into.

Remington added that reproducibility depends largely on validation of methods, so the descriptions of those methods should be very well done. The costs for data storage can be enormous. The National Center for Biotechnology Information (NCBI), which is funded by the National Institutes of Health (NIH) spends \$250 million per year for data storage. Researchers cannot sustainably provide that service; grants eventually run out.

Joachimik noted that correcting errors in the databases is important. One needs to figure out how corrections can be made. Annotation data are likely to be at least 15% erroneous. Weatherwax responded that KBase and other systems are allowing the fixing of data. Thomassen added that BER investigators have been required to follow a lot of these procedures for years.

Weyant asked to what extent one can leverage international efforts that are involved in the same types of efforts that DOE-funded researchers are. Many of the international projects and societies have data-management systems. Weatherwax said that a lot of BER's data plans use the features of international organizations. Weyant added that the problem is the continued funding of such international organizations. It is good to have a Plan B.

Hubbard commented that there is the AmeriFlux system, but BER has a diverse research ecosystem. As a result, a cyberinfrastructure for BER is needed. Weatherwax replied that the DMP is a minimum. BER has a broader view of a platform for different disciplines. A framework for such a platform and for the Department of Energy Systems Biology Knowledgebase (KBase) and for other systems is needed for them to interoperate.

Janetos said that archiving data is as important as where to do the next initiatives. Weatherwax replied that archiving data could be a topic discussed by the charge subcommittee. Thomassen added that he would encourage more discussion on that topic. Reviewers will have an opportunity to shape the preservation activities through their critiques of the DMPs.

A break was declared at 11:08 a.m.

The meeting was called back into session at 11:21 a.m., and **Gary Geernaert** was asked to discuss the activities of the CESD.

All 2014 SFA and facility reviews were completed, including two in the week prior to this meeting: the Environmental Molecular Sciences Laboratory (EMSL) Facility and the Regional and Global Climate Modeling (RGCM) SFA. All garnered approvals, and it was exciting how excellent they proved to be. The schedule for the 2015 SFA and facility reviews has been set, and all reports are upcoming. Twelve PI meetings and workshops were held during 2014. Six PI meetings and workshops have been scheduled for 2015: the North American Carbon Program workshop and Ameriflux PI meeting; Climate-Energy Model Interdependencies Workshops, Parts 2 and 3; Atmospheric Radiation Measurement (ARM) Program's Aerial Facility Strategy Workshop; Environmental System Science PI meeting; and ARM/Atmospheric System Research Facility PI meeting.

A CESD retreat was held July 8, 2014, for Division-wide team building and multiprogram CESD priority setting for the future. The retreat was built upon the CESD Strategic Plan, the unique capabilities of DOE, U.S. Global Change Research Program's priorities; the year's success stories, and collaboration with other agencies. As a group, the retreat participants agreed on four topics to pursue: urban processes and regional climate, land-atmosphere interaction, polar environments, and terrestrial-aquatic interfaces. The group reviewed facilities and instrumentation. And it selected as priorities (1) the sensitivity of existing models and uncertainty quantification; (2) the addressing of missing or inadequate data in prediction systems; (3) exploiting DOE's uniqueness; and (4) the leveraging of agency partnerships.

Descriptions of current research were offered as illustrations of areas that the Division is going to emphasize in the future:

- An investigation of statistical connections between Asia and the western United States, a present-day high-level modeling simulation
- A study of the predictability of the “climate-change hiatus” that uses initialized versus uninitialized climate models to explain why re-initialized climate models show a 16% reduction of near-term global warming
- Research to resolve why sea ice area has been declining for decades while ice age has been increasing
- Modeling of Arctic clouds to accurately represent their liquid and ice concentrations
- An analysis of how ice crystals form from aerosol particles
- A synthesis of the available literature on tundra roots and their representation in terrestrial biosphere models
- An examination of carbon uptake through warming-induced changes in temperate phenology, showing strong evidence for an earlier onset of the growing season during the past 10 to 20 years and more forest uptake of carbon
- An inquiry into the role of phosphorus dynamics in tropical forests
- An exploration of the reduction of chromium mobility by chemically reducing it to a less-mobile form

At EMSL, the new High Resolution and Mass Accuracy Capability (HRMAC) has attained its design magnetic field of 21 T, and the spectrometer and data controls are on track. The Green Ocean Amazon’s (GOAmazon’s) aerosol mass spectrometer has been deployed for a fall campaign. The Cascade supercomputer was ranked number 15 in the world in June. And NWChem, version 6.5, has been released with more than two dozen new functionalities.

Accelerated Climate Model for Energy (ACME) is a new SFA that is moving code toward higher resolution at an accelerated pace. It will use DOE leadership computers as they come online 8 to 10 years from now.

The Next-Generation Ecosystem Experiment (NGEE) in the Tropics was launched in July 2014 with a consortium of national laboratories lead by Lawrence Berkeley National Laboratory (LBNL). A vision and approach white paper was received and approved in July. A presentation about NGEE–Tropics was made to BER in August. A scoping meeting was held in Puerto Rico in September. A Phase I proposal is due on December 10. NGEE activities will be highly multidisciplinary and will provide a framework for collaboration. NGEE–Tropics will be a model-informed field study that will result in an iterative refinement of process-rich, scalable, predictive models. It will be based on field studies in the most climate-sensitive tropical geographies that provide a high scientific return on investment, and it will use a distributed network of focused research sites. Data informatics will be provided by a BER Virtual Laboratory that will provide an integrated data ecosystem for (1) critical complex systems, (2) collection and data management, (3) pattern discovery, (4) predictive models, and (5) decisions and control, all connected by data-intensive computing.

The Earth-System Grid Federation has nodes both domestic and international and supports more than 40 projects. It enables an approach to Earth-system research through the DOE BER data infrastructure.

DISCUSSION

Hubbard asked Geernaert to say more about the urban ecosystems. Geernaert replied that the carbon budget has to be considered locally. Unperturbed ecosystems are being sought out, but they are becoming rare. What is important are the urban ecosystems.

Weyant noted that NGEE work in the ACME project is full of mind-boggling new science. Keeping up with the computer hardware and software is difficult. He asked if any thought had been given to freezing the computer environment. Geernaert answered that the ACME approach is unique. The Office on Advanced Scientific Computing Research (ASCR) is developing a big part of the computational

capabilities. BER is coordinating closely with them. The national laboratories are in the center of this effort.

Zhang asked if BER should initiate a new program in urban ecology. Geernaert replied, no; it would not be a program, but it could be a priority for BER. The earlier projects were topics that were ripe for exploitation. Coastal areas are where most of the people live.

Stacey said that BER needs to be commended on its forward-thinking workshops. However, programs last about three years, and then one goes on to the next big idea. The SFAs provide a more stable funding mechanism. He asked if this structure is constraining BER in pursuing long-term research. Geernaert replied that BER may review on a three-year cycle, but a project may be of decadal scale. That gets back to the new BERAC charge: How does BER define the fertile activities of the future to guide laboratory and university efforts?

Shanks asked what ACME entailed. Geernaert answered that, during the review, BER recognized the human component as an important part to be covered. BER is looking at how to steer its researchers to the right research topics. It is charting a path forward with cutting-edge research projects.

Baldocchi asked him to be more specific about land-atmosphere interactions. Geernaert said that BER has GOAmazon. That project was not funded in the ARM program. Rather, it was funded across divisions, exploiting a variety of approaches.

Todd Anderson was asked to report on the activities of the BSSD.

In the BSSD, reviews have been completed on Plant Feedstocks Genomics for Bioenergy, Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next-Generation Biofuels, the Committee of Visitors, and Systems Biology Knowledgebase (KBase). Later this year, reviews are scheduled for the Pacific Northwest National Laboratory Foundation Genomic Science SFA, Great Lakes Bioenergy Research Center (GLBRC), BioEnergy Science Center (BESC), Joint BioEnergy Institute (JBEI), and Joint Genome Institute (JGI). Three workshops have been conducted: Research for Sustainable Bioenergy, Molecular Science Challenges Workshop, and DOE Bioenergy Workshop.

Two new positions are being posted in computational biology and microbiology.

The Funding Opportunity Announcement (FOA) for Plant Feedstocks Genomics for Bioenergy was competed, and 10 awards were made at a total \$12.6 billion for FY14–16.

The FOA for Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next-Generation Biofuels was competed with 14 awards at a total \$19.6 million for FY14–16 for new model organisms for bioenergy purposes, new functional capabilities, and novel technologies.

The awards for new plant feedstocks complement existing plant and rhizosphere research efforts at Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL), and Brookhaven National Laboratory (BNL). The new systems biology research complements existing efforts at Lawrence Livermore National Laboratory (LLNL), National Renewable Energy Laboratory (NREL), and ORNL. In addition to existing projects and ongoing efforts in the Bioenergy Research Centers (BRCs), biosystem design projects, and early career awards, it is desirable to use the Genomic Sciences Program PI meeting to encourage collaborations.

There will be three new funding opportunities: Systems Biology Research to Advance Sustainable Bioenergy Crop Development (October 1), Plant Feedstocks Genomics for Bioenergy (November), and Small Business Innovative Research (currently posted).

Money that arrived late in FY 2014 was used to fund an FOA on Bioimaging Technology Development. Five projects were funded at the national laboratories. Another FOA on this topic was posted on September 10 for university researchers.

The Office has been encouraged by the progress of KBase. It is an open-source and open-architecture computational environment for integrating large, diverse datasets produced by the Genomic Sciences Program and other sources. It allows using that information to advance predictive understanding, manipulation, and design of biological systems. It is an enabling feature for systems biology. The vision needs to be translated into practical capabilities.

The Division is providing support for individual researchers in academia to conduct team-oriented research at the national laboratories, perform technology development for systems-biology integration, exploit the cutting-edge capabilities at the DOE user facilities, and use the computational infrastructure to collaboratively link researchers with each other and with facilities. The object is to influence and enable researchers to converge on solutions to DOE science challenges.

To date, the BRCs have produced 602 invention disclosures and/or patent applications, 19 patents, 108 licensing agreements, and 1661 peer-reviewed publications. The BRC science is spectacular:

- Field trials have demonstrated the viability of reduced-recalcitrance transgenic switchgrass.
- An engineered lignin in *Populus* has been developed that improves wood degradability.
- An auto-inducible mechanism for ionic liquid resistance in microbial biofuel production has been demonstrated.
- Carbon, sulfur, and iron cycling have been integrated in anaerobic methane oxidation.
- A study has shown that fungal and plant proteins interact to allow beneficial colonization in *Populus*.
- Positron emission tomography (PET) has been used to image desert biological soil crusts and to show $^{11}\text{CO}_2$ uptake during emergence from dormancy.
- Low-dose irradiation of human cells has been shown to induce glucose flux and radiation resistance *in vivo*.
- The structure of a protein crystal was examined inside a living cell at the Linac Coherent Light Source (LCLS).

Notice has just been received that the Office of the Inspector General is auditing the BRCs.

Thirty years of macromolecular crystallography at the National Synchrotron Light Source (NSLS) was noted. The facility was shut down on September 30, 2014. The NSLS 2 just received approval for operation.

The DOE Joint Genome Institute (JGI) is looking at complex plant, rhizosphere, and microbial community sequencing; new strategies for interpreting complex genomes through high-throughput functional assays, DNA synthesis and manipulation techniques, and genome analysis tools in association with KBase; supporting biosystem design efforts for biofuels and environmental-process research; metagenome sequencing and analysis from environmental samples; and single-cell sequencing for hard-to-culture microorganisms from understudied environments relevant to DOE. It has also been asked to cooperate on joint projects with EMSL.

The JGI is a very productive facility. It has produced 67 publications since the previous BERAC meeting. In 2015, it is conducting a community science program that will cover functional genomics and microbiomes of DOE JGI flagship plants, functional diversity of microbes, microbial emission and capture of greenhouse gases in terrestrial systems, and discovery and expression of natural product pathways relevant to energy-related and environmental processes. It will also participate in the JGI-EMSL Collaborative Science Initiative in biogeochemistry, carbon cycling, and biofuels production.

DISCUSSION

Robertson noted that a number of requests for proposals do not state the size of the project. Anderson responded that there will be a pre-proposal process.

Zhang asked if the success rate for proposals at the JGI were normal. Anderson replied, yes, it is typical.

Zhao asked how the natural-gas boom will impact the DOE-funded areas and what the path forward was for visionary research in BER. Anderson replied that the *Bioenergy Workshop Report* and included the future of the BRCs. The mechanisms to be used in the future have not been thought out yet. In the longer-term challenge of the natural-gas boom, biofuels will factor into society's needs for the fuels and products derived from petroleum today. The boom will end, and society will need to move toward biofuels, so the community needs to be prepared for that eventuality.

Merchant noted that the development of technologies for bioproducts is advancing quite well.

Baldocchi commented that the scale of the use of resources like water needs to be considered. Anderson replied that the report just issued addressed that issue as do efforts at the Great Lakes BRC.

Stacey asked the Committee to review a document on cross-cutting science on crop productivity, which was provided by Schlicher. The report was on the activities of the BRCs. Individual responses from the Committee members would be appreciated.

A break for lunch was declared at 12:50 p.m.

Wednesday, October 1, 2014 Afternoon Session

The meeting was called back into session at 2:16 p.m.

Kent Peters was asked to report on the June 23–24, 2014, Bioenergy Workshop.

The original goals of the BRCs were established at a 2005 workshop. They were to develop biofuel-production feedstocks, enhance deconstruction, and to develop fuel synthesis and enabling technologies for technology transfer. Annual reviews document the success of the BRCs in meeting stated goals. The BRCs are finishing year seven of a second five-year funding period. It is a good time to define the state of the science and to identify remaining gaps and areas to inform future funding and research.

The workshop was held with 45 participants, four from industry, seven from national laboratories, and 34 from academic institutions. The workshop had speakers and breakout groups on biomass development, deconstruction of biomass, specialty fuels, and bioproduct development. A report is expected with an assessment of the current state of the science, an identification of remaining scientific and technical areas, and information and perspectives to inform BER's bioenergy program goals.

Advances that have been made in *biomass production* include the identification of new genes involved in cell-wall biosynthesis and their regulation, a demonstrated ability to genetically engineer biofuel crops for reduced recalcitrance and greater sugar yields, and the demonstration of genetic engineering to alter lignin composition and hydrolyzability. Barriers that remain in *biomass production* include further work to optimize lignocellulosic biofuel and bioproduct crops; additional work on switchgrass, *Miscanthus*, energy cane, and *Populus*; the selection of natural variants, genotype-assisted breeding, and genetic engineering for the improvement of biofuel traits; and the prioritization of traits, including reduced recalcitrance, water and nutrient recycling, and delayed flowering.

Advances that have been made in *deconstruction* include several effective pretreatment technologies; better understanding of plant cell wall structure and origins of recalcitrance; the promise of consolidated bioprocessing and engineered thermophiles; and effective enzyme farming using metagenomics, genomic sequencing, and gene synthesis. Barriers that remain in *deconstruction* include the need for standardized biomass samples to use for comparative analysis, better analytical tools for characterizing the lignocellulose and the break-down intermediates, deconstruction streams that provide for fermentable sugars as well as valorization of lignin, and the establishment of a basic toolbox for lignin catabolism.

Advances that have been made in *specialty biofuels* include engineered microbes with higher conversion efficiencies and greater inhibitor tolerance, engineered thermophiles to make lignocellulosic ethanol without pretreatment, and new tools for synthetic biology and metabolic engineering resulting in an expanded suite of accessible molecules beyond ethanol to serve as biofuels or their precursors. Barriers that remain in *specialty biofuels* include selecting the appropriate targets on the basis of meaningful evaluation of the accessible markets, methods to test thousands of variants of a pathway in a high-throughput manner, and prediction of the performance of a microbe in industrial-scale fermentation from benchtop-scale experiments.

Gaps and areas that were identified in the manufacturing of biomass bioproducts included separation technologies and the lack of cost-effective extraction of manufactured product or raw material; inadequate integration of manufacturing with the fuel-production site; inadequate compositional analysis of potential by-product streams; lack of efficient, stable, and scalable biocatalysts for desired bioproducts; lack of

efficient and economical continuous processes; lack of flexible process technology to accommodate multiple-feedstock sources; and lack of a synthetic biological and/or chemical frameworks that only requires minor modification for a range of bioproducts.

In summary, what is desired is continued support for biofuel crop development, continued support for improved deconstruction, expansion into specialty fuels and bioproducts, the replacement of petroleum as a starting material for carbon-neutral production, a pathway to aromatics through less-toxic intermediates than benzene and toluene, an infinite diversity of new products, and continued value in vertical integration.

DISCUSSION

Robertson asked whether sustainability had been part of the workshop charge. Peters replied that there had just been another workshop focused on sustainability, and the workshop subcommittee did not see a need to repeat that discussion.

Joachimiak asked if there were any overlap between the identified research objectives and the funding opportunity announcements. Cathy Ronning, Program Manager, Office of Biological and Environmental Research, USDOE, answered that the sustainability FOA is more overarching. The bioenergy workshop is highly focused on the production of fuels and by-products; the two are complementary. Stacey commented that he had gotten the impression that the discussions were focused on commercial applications. Ronning replied that what the commercial interests needed in terms of basic science was discussed. Stacey noted that, as the prices of oil and gas drop, interest in renewables may decline. He asked whether the intellectual advances will be retained by sustained funding. Peters replied that conversion can be made more efficient, and these technologies will be needed in the future.

Remington noted that there was a lack of diversity in the speakers and breakout leaders at the Bioenergy Workshop and asked if that diversity could be improved. Weatherwax said that the organizers had a long list of potential invitees who then self-selected the final participant pool. There was a broad geographic diversity. Shanks commented that metabolic engineering has been dominated by males; it has been difficult for women to break through. Young female professors *are* being named; it is hoped that they will rise to prominence in the future. Remington added that it is worth working on getting a more diverse leadership.

Sally McFarlane was asked to report on ARM and the Southern Great Plains (SGP) Workshop.

The ARM triennial review in April 2014 found that ARM successfully met the criteria to strongly support the DOE's energy, climate, and environmental mission and the goals of BER; its operations and management are at the highest level; and its processes facilitate high-impact climate research. ARM's facility management needs to actively prepare and plan for the execution of the ARM Next-Generation vision for the development of an ARM Decadal Vision white paper. It also needs to establish a user executive committee to better engage the user community in facility planning and directions, to complete the Archive Data Discovery interface upgrade to include intensive operation period data sets, and to provide a data-backup strategy for the ARM Archive to mitigate risk from catastrophic events.

In the Tropical Western Pacific, the Nauru site officially closed Oct 1, 2013; the Manus site officially closed July 1, 2014; and the Darwin site is closing Jan 1, 2015.

The Eastern North Atlantic Site in the Azores became operational with baseline instrumentation on October 1, 2013. New instrumentation was installed in 2014, and additional instrumentation is scheduled to be installed. A workshop is planned for December 2014 with local scientists and students from the University of the Azores.

A third ARM mobile facility (AMF3) has been developed and deployed at Oliktok Point, Alaska. It has been operational since October 2013. New instrumentation was installed in 2014, and additional instrumentation will be installed in 2015. Engineering flights of tethered balloon and unmanned aerial systems (UAS) will be conducted in October 2014 to plan ARM baseline UAS activities. The Evaluation of Routine Measurements Using UAS (ERASMUS) field campaign will be held in April 2015. Flights of Pilatus and Data Hawk UAS are being conducted.

The Biogenic Aerosols – Effects on Clouds and Climate (BAECC) Project was carried out from February to September 2014 in southern Finland at a site run by the University of Helsinki. Its objective was to study the links between biogenic aerosols and cloud formation. It also conducted studies of snowfall microphysics and instrument comparisons. An article for publication in the *Bulletin of the American Meteorological Society* is in preparation. The quality of the data collected is “great.”

Green Ocean Amazon (GOAmazon) is a collaboration among two Brazilian organizations, the Terrestrial Ecosystem Science (TES) program, ASR, and RGCM. Its second intensive observing period (IOP) is ongoing. A Woodrow Wilson Center Symposium on FAPESP–US [Fundação de Amparo à Pesquisa do Estado de São Paulo] will be held by the collaborating institutions followed by a one-day GOAmazon workshop. A U.S./Brazilian student workshop is scheduled for Oct 14-17, 2014, in Manaus. GOAmazon data have shown an anthropogenic influence on isoprene chemistry and an increase in aerosol concentration downwind of Manaus.

The next ARM campaign is the ARM Cloud Aerosol Precipitation Experiment (ACA PEX) from January to February in 2015. It will be conducted in collaboration with the National Oceanic and Atmospheric Administration’s CalWater2 field campaign. The Second ARM Mobile Facility (AMF2) will be used on the Research Vessel Ron Brown, and the G1 aircraft will be deployed for aerial measurements. The objective of the campaign is to observe the evolution and structure of atmospheric rivers, to observe the long-range transport of aerosols and potential interactions with atmospheric rivers, and to examine how aerosols from long-range transport and local sources influence cloud and precipitation on the U.S. West Coast.

The ARM West Antarctic Radiation Experiment (AWARE) will be conducted from October 2015 to September 2016. Its objectives are to improve the understanding of mechanisms governing West Antarctic energy balance and climate change and to assess and improve cloud physical parameterization in climate-model simulations for the coldest climate regime.

Recently, field campaigns at the SGP, Eastern North Atlantic (ENA), and North Slope of Alaska (NSA) have also been supported.

The SGP ARM/ASR High-Resolution Modeling Workshop was held May 19–20, 2014, in Bethesda, MD., to discuss how ARM data can contribute to improved modeling that requires updated parameterizations of physical processes. It would be good to couple high-density observations with high-resolution process models to provide “4-dimensional data cubes” for parameterization development and process understanding. The measurement, modeling, data, and computational challenges needed for long-term, routine high-resolution modeling at ARM sites must be determined.

The workshop was to identify and discuss high-priority scientific questions that could be addressed with such modeling and simulations; the challenges to integrating high-resolution models and observations; the key measurements needed to improve observational constraints on high-resolution models; scientific priorities in choosing model configurations and frameworks; and the computational challenges in running, storing, and processing the model simulations. The workshop attendees included 22 scientists, 6 observers from ARM infrastructure operations, and DOE program managers. Attendees were invited to submit white papers addressing the workshop goals, and the co-chairs synthesized those white paper responses at the workshop. The workshop included plenary sessions and breakout groups. The major themes that emerged from the discussions are

- In shallow convection, the representation of sub-grid convection is a challenge for climate models and is linked to climate sensitivity. Weakly forced shallow clouds are sensitive to small perturbations in atmospheric conditions, land surface forcing, aerosol properties, and entrainment rate.
- Deep convection is a key component of atmospheric circulation and cloud systems on local and large scales. The major challenges are the representation of interacting scales; timing of convection; system organization; impacts of aerosol processes; and links to the land surface.

The workshop identified gaps/needs in the areas of measurement, modeling, and data products and tools. It set a series of short-term priorities:

- The initial focus of ARM routine modeling should be shallow convection, with a longer-term focus on deep convection
- Additional profiling sites within ~50 km of the SGP central facility are critical to provide boundary-layer profiles for model forcing
- Optimization of existing land–atmosphere coupling sites and the addition of new sites are critical for studying land–atmosphere interactions
- A pilot study should be performed to optimize the design of the modeling framework
- Additional scanning radars should be deployed for 3-D cloud properties

It also set a series of longer-term priorities:

- Exploration of data assimilation to provide improved model forcing and local-scale reanalysis
- Deployment of profiling sites at about a 200-km radius from the SGP to support deep-convection modeling
- Additional capabilities for aerosol profiling

Post-workshop activities include a workshop report that was posted online September 30, 2014; infrastructure planning for ARM at the ARM data developer’s meeting in August and the data products meeting in October; discussions with land-service experts on improving measurements; planning for the deployment of four profiling sites and three land–atmosphere sites at SGP; initial planning for a modeling pilot study; and discussions on integrating ARM activities with other modeling activities.

A workshop was held about the North Slope of Alaska on September 10–11, 2014. It focused on linking Barrow and Oliktok, measurement needs, and potential links to modeling and TES programs. A workshop in the spring of 2015 will focus on the need for aerial and satellite measurements across CESD.

DISCUSSION

Hubbard asked if the 50-km profiling site were for high-density observations. McFarlane replied that it is a step toward 30-km modeling.

Leung stated that there are both weather systems developing over an area and weather systems sweeping through from distant areas. She asked how one distinguishes between the two. McFarlane answered that there was a discussion of that issue at the workshop; BER is interested in the topic.

Zhang asked if the NSA Workshop also explored the question of high-resolution models. McFarlane said that modeling was talked about at the Barrow Site and Oliktok, which are 100 km apart, and connections with the RGCM program are being explored.

Stahl asked if the current ARM infrastructure were satisfactory for high-resolution measurements. McFarlane replied that upgrades will be needed as funds are made available.

A break was declared at 3:26 p.m. The meeting was called back into session at 3:40 p.m.

David Stahl was asked to report on the Committee of Visitors (COV) review of BSSD.

The charge to the COV was to assess the processes used to create and manage the research portfolio in the BSSD of BER. The COV met on July 9–11, 2014, at the DOE headquarters in Germantown, Maryland.

The COV reviewed BSSD elements that were active since the prior COV review: the JGI and Structural Biology facilities, SFA Program Areas dealing with (1)

- Ethical, legal, and societal issues
- Genomic science
- Low-dose radiation
- Radiochemistry;

(2) university FOAs covering genomic science, plant feedstocks, radiochemistry, and instrumentation; (3) the BRCs; and (4) the Artificial Retina Project, which was completed in 2011.

The COV was impressed with the overall quality and management of the solicitation and review of proposals. The funded programs have a good balance of risky, solid, and innovative science. No serious

concerns were raised by the COV concerning consistency with priorities and criteria stated in the program's solicitations, announcements, and guidelines.

Merit reviews were uniformly conducted with an adequate number of highly qualified reviewers. In most instances, the time between issuing the FOA, submission, and decision of preproposals and proposals was satisfactory, providing investigators ample time for preparation. There was generally good documentation of the proposal review and evaluation process. The COV noted a limited number of cases of sparse documentation supporting the recommendation for funding or declination of submitted proposals.

There is an urgent need to hire additional staff. Greater flexibility and budget support for program manager and staff attendance at scientific meetings, site visits, and contractor reviews are needed. Current staff shortages and heavy program manager and staff workloads may already have impact the COV review process. As noted by the previous COV, it would also be very helpful to provide the COV with greater background information relating to FOA and SFA development, integration, and prioritization prior to the meeting of the COV. Electronic records, when developed, should be designed to facilitate the COV review and record keeping of this process.

The BSSD is a remarkably lean operation. Several program managers have exclusive responsibility for multiple essential programs. As some program managers move toward retirement, it will be critical to develop a plan for transition to new leadership. The COV was impressed with the rigor of the FOA solicitation, review, and monitoring activities by the BSSD program managers, especially considering the limited funding for the FOAs and for support staff to administer the FOAs. The COV recommends more clarification in FOA solicitations so that the topic is more focused. The COV also recommends the pre-proposal process be more selective and that a smaller number of pre-proposals be advanced to a full submission. In addition, a major concern is the ability of program managers to adequately engage the scientific community by attending meetings and holding discussions with investigators in the field.

User programs maintained by the JGI include the Community Science Program (CSP), Emerging Technologies Opportunity Program (ETOP), JGI-EMSL Collaborative Science Program, DNA Synthesis Program, and BRC Science Program.

Currently 50% of the JGI sequencing capacity is dedicated to the CSP. The COV agrees that the overall review process is efficacious, reviewers are being drawn from sources outside of the JGI, and the quality of the reviewers is typically strong. The COV also appreciates the CSP's changing emphasis from a largely sequence generator of model organisms (e.g., single microbe) to undertaking more complex projects (e.g., microbial communities), and an increasing focus on the ability to analyze and interpret the sequence data produced. ETOP has only recently (2012) been undertaken to identify new strategic partners and unique scientific capabilities. Six projects were awarded in mid-2013 from nine full proposals [out of 69 letters of interest (LOIs) received]. The JGI-EMSL Collaborative Science Initiative began in 2013 with 27 proposals submitted. This is a significant opportunity to facilitate new approaches to answer questions in the biological sciences relevant to DOE missions. The DNA Synthesis Program represents another initiative by the JGI to transition into new areas of genome-based science. Synthetic biology and biological engineering represent new frontiers in microbiology.

The COV recommends that the review process for these new initiatives be developed into a robust peer-review process that reaches out and includes outside scientific expertise. This review should include regular, documented evaluation addressing specifically whether the facility is the best use of program resources. A continued and expanded effort should be made to advertise the presence, purpose, and results of these programs to the wider scientific community.

The BRCs receive about 30% of the JGI sequencing services, and this includes the completion of large, complicated plant genomes that are generally beyond a university facility. The JGI is providing an appropriate contribution to this effort. However, JGI should continue to evaluate the core sequencing services they provide against the continuing rise in sequence capacity at many institutions and the impact this may have on future emphasis of DOE resources in this area. An external advisory process could periodically consider this question.

In regard to the relation between JGI and KBase, JGI's overlap with the development of KBase as an analytical resource needs to be conducted and monitored carefully through a formal mechanism and in a strategic manner to leverage JGI and KBase resources in the most efficient manner.

BSSD supports structural biology through programs at ANL, BNL, Cornell University, LBNL, ORNL, Los Alamos National Laboratory (LANL), and Stanford Linear Accelerator Center National Laboratory (SLAC). BSSD also co-funds the Protein Data Bank at Rutgers University with NIH and NSF.

The research community benefits enormously from these structural biology facilities. The program manager is well versed in all of these projects and remains actively involved in supporting further developments of X-ray free-electron lasers, synchrotron radiation, and neutron-scattering facilities. The qualities of the chosen referees and their written reviews are excellent. The COV members have no concerns regarding the appropriateness of the reviews or program management. The COV emphatically encourages the continued co-funding of these facilities with NIH and other agencies. Continued support of the Protein Data Bank is essential given that this data bank influences a wide range of bioenergy research from enzymology to cell biology, nationally and internationally.

The COV was concerned with the lack of substantial funding set aside for capital equipment, which prevents long-term planning of new beamline facilities or major upgrades. This is critical for SBC to remain internationally competitive. BSSD put in place a mechanism to prepare for the timely upgrades of BER-funded synchrotron and neutron experimental stations. The COV also strongly recommends that the BSSD management prepare a timely succession plan and at the same time establish a panel of experts to help prepare for both a smooth transition of leadership and for the establishment of a road map to guide future facility development and operation.

The COV was very supportive of the shift from single investigator to SFAs to encourage collaborative, multidisciplinary research within the national laboratories. There are currently 18 SFAs funded by BSSD in the national laboratories in ethical, legal, and societal issues (ELSI), genomic science, low-dose radiation, and radiochemistry. With the exception of KBase, the 18 projects reviewed by this COV existed at the time of the previous review. The COV was supportive of the KBase solicitation and review process and recommends this general process serve as a template for the solicitation of future SFAs. A well-defined and documented system was employed to solicit proposals from the national laboratories, obtain written reviews from high-quality reviewers, conduct reverse site visits, make awards and declinations, and obtain budget revisions. However, the decision process could be better documented. The program managers are doing an excellent job managing the SFA programs. Specifically,

- In ELSI, now focused on upcoming societal challenges related to bioenergy and nanoscience, review documents and communication among PIs and DOE program managers were very well organized. This documentation was extremely useful, and similar documentation should be provided for each SFA in future COV reviews. The COV encourages BSSD to continue support for ELSI as an integrated component of ongoing scientific programs.
- KBase is scientifically exciting and at the cutting edge of the discipline. This is high-risk, high-potential-impact research but also has a significant service/outreach component to ensure the methods and tools developed are actually used. It is unclear what mechanisms have been put in place to communicate with possible users, interface with DOE JGI, and/or involve other FOA grants; and there are significant challenges to achieving a "one stop" computational resource. There has clearly been a very significant involvement of program staff to ensure that KBase remained an appropriately mission-oriented project. However, the balance of plant to microbial emphasis within KBase should be revisited. The best mechanism for evaluating tools is to solicit reviews by potential or current users, and the best mechanism to measure impact is to count peer-reviewed publications that cite or acknowledge KBase. A plan should be put in place to provide necessary computational resources (e.g., flexible cloud compute allocation) for any tools developed under this program that are both successful and computationally intensive.
- Biofuels are a major part of the SFA research portfolio, and the research complements the BRCs, which are managed separately. The scientific quality and breadth of these programs is very impressive. The current SFAs in this program are of appropriate scientific depth, of high overall

quality, and well managed. However, the COV was divided on the potential for the various biofuel-related projects to ultimately benefit the nation, which may reflect the lack of a high-level rationale for support of the individual projects and the expected synergy among projects.

- The Foundational Genomic Science SFAs cover varied aspects of microbial ecology and are collaborative and interdisciplinary and use state-of-the-art techniques and novel approaches. These projects are among those leading the field in environmental microbiology research. However, it was very difficult to determine the numbers of PIs involved in each project, how the projects related to each other, and who produced the summary of the review panel.
- The Low-Dose Radiation Program's productivity has been high, and the program is unique in addressing issues central to potential health effects from environmental, occupational, accidental, and medical exposures to ionizing radiation. However, its budget was reduced from \$21.7 million to \$6.2 million in the time span covered by this review (2011–2013). The COV is concerned that the absence of new low-dose SFA solicitations in this review period will compromise the future of this program. The COV recommends exploring the possibility of interagency co-funding or international coordination to recover momentum and expand efforts in this research area. New initiatives in the low-dose program are essential for retaining the balance between federal laboratory and university efforts.
- The radiochemistry and imaging SFAs are well organized and managed. The review and award process is clear, and there is a thorough review process for all proposals with consistent high-quality reviews. The program manager has each SFA well documented and is in close communication with the PIs. All SFAs are consistent with the DOE mission.

The SFAs' triennial reviews appear to have been well managed in all aspects. Given the staff shortages within the BER Program and limitations in the travel budgets, the detailed interaction with PIs is commendable and additional staff to replace current vacancies will assist future reviews.

Some general recommendations were made about the SFAs: A formal, documented, and reviewed process for the creation of new SFAs should be developed. There should be a clear process and documentation of the decision process for redirecting or terminating an SFA. There is some natural redundancy across and within SFAs funded at national laboratories, and it is not clear that any mechanism exists to prevent redundancy and promote dialog between related projects; BER management should develop mechanisms to produce such dialog.

Seven FOAs were targeted to the university community.

- The joint DOE–USDA [U.S. Department of Agriculture] Plant Feedstocks for Bioenergy Program was seen as strategic and a powerful way to leverage funds, interest, and expertise between DOE and USDA. The COV was particularly impressed with the rigor of the review process for the three Plant Feedstock FOAs and felt that the proposals selected for funding were the most meritorious proposals. The program manager was in regular contact with the awardees through e-mail correspondence, annual reports, scientific meetings, and the annual awardees meeting.
- The focus of the three Biosystem Design FOAs is distinct, and the program has evolved over time to address new scientific areas and to attract new investigators to DOE. The program appears to have a balance with respect to breadth, although tradeoffs between breadth and depth may occur when soliciting larger, multidisciplinary, longer-duration projects. The success rate for proposals submitted to these FOAs was highly variable, ranging from 9% to 29.4% (average: 14.8%). It would be useful to articulate a vision to connect/translate the systems biology aspects of the portfolio to the Plant Feedstocks Program portfolio. The selection of only one project each per organism type in the Biosystem Design FOA may not give sufficient depth to cover this field.
- In nuclear medicine, the Low-Dose Radiation Research Program had no FOAs from 2011 to 2013; this was seen as a major weakness. The Radiochemistry and Instrumentation Program has suffered severe cuts in funding. An appropriate level of funding to both universities and national

laboratories is needed to maintain essential training and workforce development in key radiochemistry areas.

In general, a more focused solicitation and/or more rigorous screening of pre-applications is advised so the funding rate is elevated to 20 to 25%. The COV was concerned about one project (Microbial Ecology, Proteogenomics, and Computational Optima, Harvard Medical School) that receives a significant amount of funding per year without substantial review, which did not seem to efficiently serve the BSSD mission or be especially well thought out.

Oversight of the BRCs appears to be appropriate for the level of investment in these centers. The BRCs in general showed both strong oversight and strong site-level management producing excellent and well-organized proposals, reports, and reviews. A decision was made to request renewal proposals from each of the three teams in 2012. Reviewers included experts in relevant areas of science with a broad view of the field, capable of judging the potential for successful impact of the proposed research. The productivity of the Centers was judged to be appropriate to excellent. The COV recommended maintaining appropriate review and oversight to ensure that BRC research remains focused and consistent with the funded BRC research programs and not overlapping or competing with other funded programs, including related SFA initiatives. Also, a unified strategic plan should be developed for the BRCs and biofuel SFAs.

Although there was no BSSD review of the Artificial Retina Project, the COV felt it appropriate to recognize the success of this project. Since termination of the project in 2011, a commercially available artificial retina received FDA approval for broad clinical use in 2013 and was ranked as the number one medical technology breakthrough for 2014, an example of an important biomedical outcome that would not have occurred without the commitment and resources of the DOE.

The COV felt that the support for conferences and workshops (5 in 2011, 12 in 2012, and 9 in 2013) was a good use of discretionary funds and supported a worthy range of meetings on topics relevant to DOE.

DISCUSSION

Shanks said that the COV had done a great job. It made a lot of recommendations, but they were not prioritized. She asked how the report will be used. Stahl replied that the Subcommittee tried to give equal weight to the recommendations; certain topics (like program-manager travel) were emphasized by repetition.

Merchant said that one comment on principal investigators at SFAs indicated a lack of gender etc. diversity. It might be something to think about. Stahl said that the COV made recommendations on that topic in the report.

Robertson asked if there were any other areas besides travel restrictions that were legacies of the previous COV. Stahl replied that nothing stood out. Travel funding is complicated by the budget cycle. Under a continuing resolution, travel is only fractionally allocated. He expressed the hope that this report would help. Weatherwax replied that every COV report comments on this problem; the repetition does not hurt. Remington commented that, at this stage, the level of travel funds is acute, not chronic. The program managers need to do due-diligence visits.

Stacey suggested an editorial change to the mention of personal information in a few places and then called for a motion to accept the report. Merchant so moved and Zhang seconded. The vote was unanimous to accept the report.

Stacey pointed out that a progression of decisions has to be made for things to show up in the budget. He requested comments on the BRCs and how they might go forward. Wall noted that a lot of money has been spent on the BRCs and a skilled workforce had been developed, especially among young workers. She questioned whether it was important to maintain that workforce or would they to be told that they are no longer needed.

Ehleringer stated that a holistic approach to workforce development was needed.

Shanks said that the level of detail needed to evaluate some technologies is very high. An impartial evaluation of these technologies is needed.

Baldocchi noted that BER is dealing with complex systems and with basic questions about water availability and competition between biofuels on the one hand and food and fiber on the other.

Schlicher called attention to the separation of DOE and industry and pointed out that the transportation industry has relied on ANL for modeling for a long time.

Braam said that, after 10 years, it might be time to open up competition for the BRCs and see who else could contribute.

Janetos said that research must consider not only the efficiency with which conversion can be made but also the coupling to the land and water. The U.S. ethanol policy caused a food-price shock around the world. DOE has tools for analyzing economics and physical effects. Opening up the discussion to others might be good. Weyant agreed that it might be a good time to look at other inputs. A public accounting process and a health an environment analysis are needed. The science changes, and the changes in environmental impact may be large.

Joachimik said that the needs of society for research need to be reassessed. The science should also be integrated. Where the science is right now and what type of research should be conducted should be assessed.

Shaver said that the systems-science approach has affected his research tremendously. It is very significant. The systems that are being talked about should be defined in a broader manner. The bigger problem is the bigger system.

Robertson noted that two useful points have come up in considering the BRCs: Is the whole bigger than the sum of its parts? Is there sufficient sustainability as broadly defined? This Committee needs to think about these issues in a broader way. It needs to consider all the environmental services.

Zhao said that every funding level will have problems. A balance needs to be achieved. The whole needs to be considered, not the sum of the parts.

Hubbard said that there is some resistance going on (e.g., in the workshops). To have all of those pieces of information is important.

Stacey said that, at the Bioenergy Workshop, it was brought out that product development at the BRCs is very different from that in the petroleum industry. Basic questions of biology and environment need to be addressed by BER. The budget cycling means that what was worked on in the 1970s is being reinvented. Today, the pressing issues are climate, population, and water use. Systems science cannot be the systems science of everything. There has to be some fractionation of topics so that one can get one's hands around a given topic.

Janetos said that BER has to begin to understand how ecological principles play out over landscape.

Schlicher said that one has to support man-on-the-moon projects as well as the killer experiments.

Stahl said that it seems that climate-change and land-use issues have to be combined.

Baldocchi noted that DOE has the skills to replace petroleum.

Merchant said that it sounds like the Committee was agreeing to establish a working group to consider where the BCRs should go after 10 years. It made sense 10 years ago to take specific approaches. Now it should be possible to tell what approaches are workable.

Weyant stated that one needs to have people who know about climate change *and* land and water issues.

Wall said that one of the tasks that the Committee was being asked to undertake is to predict the future and how people will live in it. It needs to consider questions like: What if roads collected sunlight for energy generation? There is a lot of biology that is not known but will be important.

Merchant said that scientists do not have a crystal ball to tell them what the problems will be in the future. However, it is known that basic science will be needed to deal with those problems.

Janetos pointed out that some of the facts about the future are understandable. The natural-gas boom is not going to last. A platform needs to be erected on which projects can be placed but can be altered as the conditions change. It is a broader conception of fundamental science.

Baldocchi noticed that science is dealing with a lot of feedbacks and other complexities. Schlicher added that there are a lot of models out there that could identify the major barriers and how to get around

them. She appreciated everyone's reading the proposal that she had circulated and also appreciated that people are willing to look at where the BRCs should go.

Stacey asked for introductory comments on the new charge. Robertson said that four areas need to be considered:

- atmosphere/climate,
- subsurface biology,
- ecosystems, and
- modeling.

Stacey asked how the Committee should proceed.

Hubbard suggested that the Committee should consider the basic topics and fill in the subcommittees with experts and other topics. The Committee needs to consider BER's field sites and other resources and see what else is needed to challenge models.

Ehleringer stated that the Committee needed some clarification about the scope with which it is to deal. Stacey suggested asking Weatherwax to provide such clarification on the following day of the meeting.

Stacey opened the floor to new business. Weyant asked how the agenda was set. Stacey said that it was done in consultation. Any Committee member can send any suggestions to the chair.

Stacey opened the floor to public comment. There being none, the meeting was adjourned for the day at 5:07 p.m.

Thursday Session, October 2, 2014

The meeting was reconvened at 8:32 a.m.

Andrzej Joachimiak was asked to give a science talk on the use of light sources and structural biology in helping to combat antibiotic resistance and infectious diseases.

Biological systems are very complex. It is not understood how molecules affect gene expression; the same blobs seem to reorganize proteins in different ways. An understanding of the biology rests on macromolecular structures and progresses through conceptualizing the macromolecules, determining their functionality, and deducing their mechanistic pathways. Nano and micro X-ray crystallography is a major tool in studying these molecules.

Biology user facilities at U.S. synchrotrons and light sources support basic research in bioenergy, environmental studies, and human health. In the past year, the synchrotrons and light sources have had the most users ever, and a large fraction of them were biological researchers. In 1995, about 10% of structures were solved by synchrotron radiation; in 2013, about 91% of the structures were thus solved.

At the Advanced Photon Source (APS), a multi-bend achromatic lattice is being installed to improve the beam's spread and smoothness. If APS is upgraded, that will produce a brilliance that is 2 to 3 orders of magnitude greater than any other source in the world. Because radiation damages the sample crystal, a 1-mm line-focus beam is used to allow atomic resolution. It also allows one to measure smaller molecules and crystals.

Because the sample must be in the form of a crystal, a facility was built at the APS to prepare crystals suitable for synchrotron analysis. That facility is a component of the Advanced Protein Characterization Facility to which researchers can now e-mail a sequence and within a week have a characterization of the protein. The massed capabilities of this facility allow a protein structure to be solved for the first time from a single-cell genome of an uncultured marine sediment *Archaea*, showing that one can perform detailed characterizations of enzymes from native subsurface microorganisms without requiring growth in pure culture. This capability is not available through any other techniques and promises (1) an

understanding of key common transformations in the environment and (2) the identification of new enzymes for biotechnological applications.

In bioenergy research, the light source is used to investigate the deconstruction of lignin. Bacteria use a complicated system to metabolize lignin. A temperature-dependent lignin-binding profile was developed for 17 crystal structures to provide clues about ligand binding during lignin deconstruction.

In human-health research, the light source has been used to study such infectious diseases as Ebola. Structure-based screening is critical to understanding the Ebola virulence. The high mortality of the Ebola virus is caused by its ability to disrupt the body's immune response to the infection. Understanding that mechanism is crucial for the development of treatments, so researchers

- Determined the crystal structure of Ebola VP24 in complex with human KPNA5;
- Developed templates for antiviral drugs for viral targets; and
- Conducted structure-based *in silico* screening, biochemical, and structural characterization of small molecules that target VP35.

Another line of research addressed the rising antibiotic resistance in the United States. The annual domestic impact of antibiotic-resistant infections on the U.S. economy has been estimated at \$20 billion in excess direct health-care costs. Additional costs to society for lost productivity are as high as \$35 billion per year. Concerned about this problem, the President's Council of Advisors on Science and Technology recommended

- Improving surveillance of the rise of antibiotic-resistant bacteria,
- Increasing the longevity of current antibiotics, and
- Increasing the rate at which new antibiotics, as well as other interventions, are discovered and developed.

One such bacterium is carbapenem-resistant enterobacteriaceae (NDM-1), which has emerged in more than 40 countries worldwide. An effort was made to understand the emerging disease and to develop drugs to combat it. The NDM-1 structure was determined and compared with other mannose-binding lectin (MBL) structures. The active site was located in the middle of the molecule between two beta sheets. That active site has a binding pocket that is twice as big as those in other proteins. NDM-1 seems to specifically recognize the β -lactam moiety; the rest of the ligand is recognized by mainly hydrophobic residues in the pocket. The crystal structure was determined with hydrolyzed ampicillin, and the active site was simulated. The simulation showed that an oriented hydroxide ion (or water molecule) serves as a general base to accept a proton from a bulk water molecule. A high-throughput screening of approximately 50,000 compounds against purified NDM-1 enzyme revealed several inhibitors with micromolar IC_{50} s [the concentration of a drug needed to inhibit a biological process by 50%].

Unfortunately, there are 12 naturally occurring variants of NDM. Kinetic measurements are being carried out for the five most common strains in the United States.

The question arose whether one could develop a drug that was effective against NDM-1.

Inosine 5'-monophosphate dehydrogenase (IMPDH) is a universal and essential enzyme found in all three kingdoms of life. Inhibitors of bacterial IMPDHs are known to inhibit pathogenic bacteria. Human type II IMPDH is actively targeted in drug development programs for immunosuppressive, anticancer, and antiviral chemotherapy. Ribavirin and mycophenolic acid (MPA) are known inhibitors of the human IMPDH enzyme. Several parasites have been targeted with inhibitors. Most drugs that are successful in the inhibition of mammalian IMPDH are far less effective against the microbial forms of the enzyme. The goal was to exploit differences in order to design drugs that target microbial IMPDH.

The IMPDH reaction mechanism is complicated. Nevertheless, a novel NAD⁺-binding mode [nicotinamide adenine dinucleotide] was found in bacterial IMPDH that provided a rationale for the binding of inhibitors. However, when one compares IMPDHs from four different species, they show very different sensitivities to inhibitors. *C. parvum* inhibitors worked in some species and not in others.

Multiple structures of IMPDHs from seven pathogenic bacteria have been determined, including structures of the protein-inhibitor complexes. These structures provide the basis for exploring the inhibitor

selectivity and offer a potential strategy for further ligand optimization that can be used to design more-potent inhibitors of bacterial IMPDHs.

In summary, high-throughput (HTP) technologies in molecular and structural biology can (1) be applied to complex problems (such as antibiotic resistance, human, animal, soil, and marine microbiomes) and (2) provide proteins for functional and mechanistic studies as well as studies of structures of proteins, protein/ligand, protein/protein, and other complexes that are functionally important. Advanced structural studies (such as obtaining structures of protein complexes or more precisely identifying substrates, products, and inhibitors of enzymes) are expected to contribute to the understanding of metabolic pathways, guide their engineering, and contribute to the development of new treatments and drugs. Basic research is essential for understanding antibiotic resistance and developing new approaches to antibiotic therapies as microbes evolve to evade existing antibiotics. Combining genomic data with biological observations and HTP structural-biology technologies can help advance our understanding of microbes and microbiomes and their evolution, adaptation, and interactions. Exploring the microbiomes' genomic potential may result in discoveries of new biology, chemistry, and metabolic pathways.

DISCUSSION

Stahl noted that one thing that had not been talked about was the discovery of new antibiotics. Joachimiak replied that his group is collaborating with a group that is studying metabolic pathways in bacteria that will synthesize unusual compounds. Work has also been done on (sort of) fighting between different bacteria that can be exploited. You can also use systems in which individual genes are kept under control and one can test whether the conditions can be overrun by the expression of particular genes. In macrophages, tryptophan is essential for survival, which provides another pathway.

Judy Wall was asked to report on the Workshop on Molecular-Science Challenges that she co-chaired.

Molecular science underlies all of BER's work, and BER deals with systems across a broad range of physical scales. The question is whether one can get information from one scale that can predict behavior at other scales and improve the models. A Workshop on Molecular Science Challenges was held May 27–29, 2014, with 22 participants who did not speak the same scientific language. The workshop charge was to understand the molecular systems and processes that underpin BER program goals, integrate across the breadth of spatial and temporal scales of the BER research areas, take advantage of resources of the DOE national laboratories and facilities, identify challenges and opportunities, describe research pathways to overcome barriers in BER-relevant molecular science, and plan for a time horizon from 2014 through 2024. The workshop had a keynote address, breakout sessions, and a writing session.

The keynote address on carbon and contaminants in the critical zone by John Chorover looked at chemical interactions, biological processes, and physical processes. The breakout sessions were on atmosphere–land surface interactions, near-surface and below-surface interactions, and synthetic science and engineering. The cross-cutting themes that emerged were

- A skilled workforce and training are needed
- Iterative interactions must occur with the modeling community
- More access is needed to computational power
- There must be an expansion in observation capabilities
- Every scale exhibits heterogeneity
- Guidelines for parameterization of heterogeneous variables are needed for predictive models

For atmosphere–land surface interactions, the decadal vision was to determine how to meet the increasing need for energy without causing harm to the Earth's climate and environment. This vision should be attained by focusing on

- *Exchange processes between land and atmosphere:* Molecular-scale data should be integrated into macro- and global-scale modeling to elucidate atmospheric impacts. The chemical and particulate emissions and depositions between land and atmosphere should be identified and

quantified. Whether there are unidentified phenomena operating across interfaces should be determined.

- *Aerosol links to radiative balance, cloud formation, and precipitation:* A global-level predictive modeling ability for cloud formation and lifetime, for anthropogenic and biogenic emissions, and for the effects of clouds and emissions on the Earth's radiative balance should be obtained. A theoretical understanding of water interactions with different types of aerosols should be developed. The mechanisms and rates of release of biogenic emissions from soil, natural waters, plant surfaces, and other sources through the action of microbes and other biological sources should be determined.
- *Terrestrial ecosystem impacts from transfer of water, gases, organics, and particles to and from the atmosphere:* The molecular mechanisms of chemical and biological cycling of minerals and transformations of organic compounds should be elucidated. The effects of land-surface-use changes on energy, particulate emissions, and water transfers with the atmosphere should be ascertained.

Attaining these goals would require (1) networks of sensors to probe the length and time scales that govern transport and reactions among air, soil, and water and to elucidate the effects on the development and growth of plants and microbes; (2) sensor networks tunable to different resolutions to detect physical or chemical events; (3) sensors of low-cost and long-duration; (4) analysis of natural samples at ultralow concentrations and low sample volumes; (5) high-speed distributed data archives; and (6) multidisciplinary training.

For near-surface and below-surface interactions, the decadal vision was to quantitatively understand biogeochemical processes and their interdependences at molecular to ecosystem scales under changing climate and land-use patterns. This vision should be attained by focusing on

- Linking genes with phenotypes in microorganisms and plants
- Predicting changes in microbial and plant population composition and structure caused by dynamic changes in the environment
- Predicting microbe–microbe and microbe–plant community interactions at molecular to millimeter scales
- Determining the influence of pore size, bacterial, and mineral surfaces on the properties of water and aqueous reactions
- Establishing electron shuttling/transfer mechanisms in complex natural systems
- Defining enzyme functions at the pore and ecosystem levels
- Developing techniques to detect, characterize, and monitor below-ground hot spots/moments
- Establishing paradigms to scale molecular- and pore-scale processes to ecosystem and landscape scales

Attaining these goals would require (1) real-time imaging at nanometer resolutions with element speciation and parts-per-million sensitivity; (2) ultra-sensitive, high-throughput spectroscopy that can analyze ultra-low volumes and masses to determine structure and composition at the pore scale; (3) noninvasive, high-throughput, sensitive techniques for probing physiological responses; (4) sensors for detecting and monitoring *in situ* subsurface processes in real time at length scales of microns to meters; (5) expandable molecular modeling tools and more computational power; and (6) thermodynamic constants for critical species.

For synthetic science and engineering, the decadal vision was to take a different approach in which electron transport is a major driver and to develop “Newtonian-like” rules that underlie the interaction and evolution of biomolecules and processes. This vision should be attained by focusing on

- Electronics principles (the management of energy transduction by cells engineered to produce a nonnative function, for example) affecting biofuel production by bifurcating electrons
- A multi-scale, three-dimensional observation of biological cellular events to identify key players
- Visualizing, conceptualizing, and testing of molecular networks in a relevant time scale

- Observing and measuring the impact of these molecular systems at successively linked system scales

Attaining these goals would require (1) developing visualization tools for macromolecular structure and dynamics of the cell; (2) determining the positions of subcellular structures and distribution of metabolites and ions; (3) developing experimental and computational techniques capable of identifying individual macromolecular and small-molecule species in the cell; (4) deriving a time-dependent 3-D view of the cell to follow the evolution of systems; (5) creating computational methods to simulate, at the molecular level, the mechanisms of enzyme functions and macromolecular machines; and (6) developing multiscale computer simulation methods that would lead to systems-level prediction of the effects of molecular-level engineering.

DISCUSSION

Stacey asked what electonomics was. Wall replied that it is the rules of electron transfer and the roles of electron transfer in biological processes.

Joachimiak asked how one can use “omics” for producing products. If one has a compound that is not being recognized, how does one find the impact of that on enzymes? Wall replied that any time one is diverting resources from making new cells in a microbial setting, the cells will slow down in growth. The cell will try to get rid of the component that is draining energy. It is of no matter if the cell recognizes the compound as long as it recognizes the slowness of growth. Anything that is growing faster will survive. One can track it and make the construct. One has to convince it to take certain pathways, or one can rely on evolution to drive new pathways. If there were good enough annotations of genes, one could do engineering.

A break was declared at 10:10 a.m. The meeting was called back into session at 10:20 a.m.

CHARGE DISCUSSION - CONTINUED

Weatherwax noted that there are a lot of ways to organize BER’s program. It comes down to cross scales, do observations, and collect data. BERAC has identified key challenges between disciplines, scales, geographic areas, and organisms. The question is, where are the key areas that should be studied and where experiment and modeling should be integrated? What are the priority science areas to address the gap between laboratory and field? Hubbard noted that the report on the virtual laboratory has identified some of those areas. Weatherwax said that the report and workshops have touched around the edges of the field setting.

Baldocchi asked what the other degrees of freedom were, noting that whole systems (e.g., continents) are not looked at. That is another data level.

Remington said that, in the National Ecological Observatory Network (NEON), there are tons of information from decades of work. Efforts by DOE and other agencies need to be leveraged. Janetos added that NEON is the only program to look at different scales. The charge leaves out the biggest driver of changes in the various cycles: humans. What needs to be figured out is how to cope with human changes of land use, water use, hydrology, etc. Remington noted that land use was the first thing that had been cut when there were restrictions on the budget.

Ehleringer pointed out that BER was to study the carbon cycle. Computer models have been developed. Critical systems (i.e., in the tropics and the Arctic) are being looked at with free-air carbon dioxide enrichment (FACE) projects. Understanding the carbon cycle requires understanding the urban ecosystem. That is where one can influence design and carbon cycling.

Leung pointed out that mountains are important to the atmosphere, water, and other critical processes that propagate to other regions.

Hubbard said that the carbon cycle is central. If observatories are to be developed, there are other interests in BER (hydrology, water quality, etc.). These gaps need to be filled in, and connections need to be made. Wall added that there are strong arguments for a lot of settings. In an urban setting, one can measure the hydrology there, also. Climate change is not off in the Arctic; it is here now, and affects how one takes showers in the morning.

Baldocchi returned to the topic that the big issue is scale. One needs to address it in a multi-scale manner. It is important how one pulls the scales together and understands the basic biology and physics.

Shanks pointed out that there are various energy sources (e.g., petroleum and biomass). The ARM sites are not in the big band of the country that affects climate change, between the Great Lakes and the East Coast.

Shaver said that many of the projects that are operating are in managed systems. Scaling is a challenge. Basic procedures (e.g., turnover rates and organism longevity) need to be understood and generalized.

Stacey warned that the Committee needs to be more specific in its recommendations.

Janetos said that if the ultimate purpose of the charge is to improve predictability, there are two ways that one might accomplish that: One is to get a better idea of the sensitivity of the various systems, mostly the terrestrial system but also at the interface between the land and the climate system, where the processes are not understood well enough to model them. Another purpose is to understand the magnitude of the perturbation and the effects of scale. What is the optimal strategy to deal with these questions? Both the Earth system and the fluxes that it experiences need to be considered.

Baldocchi said that something needs to be done at the scale of the entire United States. Maybe that is why the mountains and cities have been omitted. Stacey said that that addresses the *where*; he wanted to know the *what*.

Leung pointed out that different timescales needed to be looked at, also.

Stahl said that the carbon cycle is only one of many cycles that are interconnected. Perhaps a couple of cycles could be selected to investigate.

Wall suggested studying the bread basket area of the United States. The nitrogen cycle there is important but not well understood. Nitrates cause acid rain, for example.

Ehleringer said that geochemical processes should be coupled with the carbon cycle. Important areas are from Missoula to Tucson and a few cities on the East Coast. There are not any pristine sites anymore. There are ripple effects that occur across urban areas.

Stacey said that he would like to see urban centers compared with mountain environments.

Shaver suggested that sustainability may be a topic to focus on.

Hubbard suggested that someone from NEON be invited to address this Committee. Remington said that there is a lot of information about the planning, operation, and management of NEON that could be passed on. Stacey agreed that there is a lot of expertise available outside this Committee (e.g., from NEON). A small workshop might be a good idea. He was not the one to lead such a workshop. One or two people would be needed to get a subcommittee together and start to organize such a workshop. Ehleringer volunteered himself and Janetos. Janetos did not object. Stacey called attention to the need for diversity. Integration and cooperation among national laboratories needs to be addressed under this charge, also. There are a lot of opportunities here, and diversity would be important.

Stacey re-opened the BRC discussion. He pointed out that BERAC cannot direct BER to do anything. It can only offer advice. There seemed to be consensus that the BRCs have been successful and that this is a good opportunity for reevaluation and reassessment.

Stacey opened the floor to new business. Remington said that she would like to see a discussion at a future BERAC meeting about encouraging diversity.

Stacey opened the floor to public comment. There being none, the meeting was adjourned at 11:08 a.m.

Respectfully submitted,
F. M. O'Hara, Jr.
Recording Secretary
October 22, 2014