Draft Minutes
Biological and Environmental Research Advisory Committee
October 28–29, 2013
Hilton Washington, D.C./Rockville Hotel & Executive Meeting Center
Rockville, Md.

BERAC Members Present

Gary Stacey, Chair
Dennis Baldocchi
Judith Curry
James Ehleringer
Andrzej Joachimiak
L. Ruby Leung
Gerald Mace
Sabeeha Merchant
Joyce Penner
James Randerson
Karin Remington
G. Philip Robertson
Gus Shaver
David Stahl
Judy Wall
Warren Washington
Minghua Zhang
Huimin Zhao

Monday, October 28, 2013
Morning Session

The meeting was called to order by Chairman **Gary Stacey** at 9:00 a.m. At his request, the Committee members introduced themselves and updated the Committee on their current research activities.

Sharlene Weatherwax was asked to update the Committee on the activities of the Office of Biological and Environmental Research (BER) of the Office of Science (SC) of the Department of Energy (DOE).

A big change is the Department's structure, with the addition of the Secretarial Counsel. Several additional offices have been added to SC. Environmental Management has been moved from the National Nuclear Security Administration to the Office of Management and Performance. Patricia Dehmer is the acting director of SC.

Stacey asked if these changes were just operational or whether they would be reflected in the Congressional appropriations. Weatherwax said that the appropriations normally do not go down to this level of detail.

The previous fiscal year was just closed out. There is not an approved budget for FY14, yet. There is a great disparity between the Senate and House markups. It is unclear when the joint conference will occur. The government is working under a 3.5-month continuing-resolution at the House mark (the lower of the two funding levels). Some things have to be put on hold and deferred. An attempt is being made to manage the portfolio for maximum flexibility in the future budget.

Stacey asked what budget the Department was currently acting under. Weatherwax replied that every DOE office is being held to the FY13 sequestered budget, which is essentially a 20% cut. Other agencies are operating at different levels.

New personnel hired for the Office include Jay Hnilo, a program manager in the Climate and Environmental Sciences Division (CESD) with responsibility for explore opportunities for data integration and modeling; Andrew Flatness, a science assistant in CESD for helping on logistics, workshops, and conferences; and Jay Fitzgerald, an American Association for the Advancement of Science fellow in Biological Systems Science Division (BSSD). Other positions are vacant and frozen until there is more budget clarity.

The United States and DOE have been involved in the Atmospheric Research 5, Working Group 1 (AR5 WG1) of the Intergovernmental Panel on Climate Change (IPCC), leading reviews and authoring reports.

DOE laboratories won 28 R&D 100 awards in 2013. BER-related awards were won by Lawrence Berkeley National Laboratory for analytical instrumentation and by Pacific Northwest National Laboratory for their developments in analytical instrumentation.

A new charge is being issued to BERAC for a committee-of-visitors review of the BSSD to review the processes used by BSSD to manage its research programs and its user facility, the Joint Genome Institute (JGI).

DISCUSSION

Stacey said that these cuts in budgets affect people's lives. A 20% cut is draconian.

Robertson asked whether the cutbacks at Oak Ridge National Laboratory (ORNL), for example, affect BER activities. Weatherwax replied that the cutbacks are accelerating the ramp down of research, but no project has been terminated. There are some personnel impacts, but they are not great.

Stacey observed that science seems to be being de-emphasized. He asked what "hub-ifying" means. Weatherwax responded that all of science is still at the table in scheduling and budgeting. SC is not being de-emphasized. The Secretary appreciates the need for science research. The Department may be looking at more collaboration. The Secretary wants an assessment of the structures of the national laboratories and the hubs see if more integration is possible.

Wall asked how the removal of science education to the Department of Education has progressed. Weatherwax stated that BER did not conduct any of the educational activities that were moved. The office that is in charge of education activities is operating under the new guidelines.

Robertson asked if there had been a nomination for the director of SC yet. Weatherwax said that there are a lot of vacancies that require Congressional confirmation. She did not know how that selection was going. Dehmer has been in this position before and is capable and confident in it.

Stacey asked what budget planning the Office was doing. Weatherwax replied that funds to national laboratories are planned for by the laboratories themselves. That is where impacts on people and programs occur. The Office has to plan for a number of potential budgets. That is where input from BERAC is useful; a lot of community input is received. Travel budgets have been heavily impacted.

Randerson noted that another major activity of BER was the development of the Community Earth System Model, which is being used in AR5 for mitigation and other activities.

Stacey noted that user facilities are highly valued by the community. Weatherwax assured him that they are protected.

A break was declared at 10:26 a.m.

The meeting was called back into session at 10:59 a.m., and **Minghua Zhang** was asked to report on the Committee of Visitors (COV) assessment of the Climate and Environmental Sciences Division (CESD) of BER.

The COV was charged with assessing the efficacy and quality of funding processes, the effect of the award process on portfolios, and other criteria. The programs and facilities reviewed included the Atmospheric System Research (ASR), Earth System Modeling (ESM), Regional and Global Climate Modeling (RGCM), Integrated Assessment Research (IAR), Terrestrial Ecosystem Science/Carbon Dioxide Information Analysis Center (TES/CDIAC), Subsurface Biogeochemical Research (SBR), ARM Climate Research Facility, and Environmental Molecular Sciences Laboratory (EMSL). The COV also looked at the cross-cutting themes of facilities, interagency coordination, workshops and initiatives, and science focus area (SFA) management and the CESD strategic plan.

The COV reviewed documents from all parts of the funding process. It also received presentations from and held discussions with program managers and other BER personnel.

The COV had three general findings:

- The CESD program managers were knowledgeable, dedicated, energetic, and committed to managing their programs and seeking solutions. There is great communication and coordination among the program managers in CESD.

- The solicitations, proposal reviews, and award decisions are rigorous. Communications with the investigators and feedbacks to the proposers were well documented. Funded projects were tracked closely. The award decision and management processes were appropriate and effective.
- The CESD programs are nationally and internationally respected; many are unique. The selected investigators and teams are world-class quality.

The COV had five general recommendations:

1. Funding to the national laboratories has been shifting to large SFAs so that complex questions and large problems can be attacked more effectively. The COV recommends that CESD maintain flexibility and an appropriate balance of funding to allow both SFAs and exploratory or cutting-edge research by individual principal investigators (PIs) at the national laboratories. The COV also recommends that CESD consider options for reducing the administrative burden of the SFA reviews while still maintaining the quality of the research program.
2. The COV considers the current overall balance of laboratory and university research to be appropriate and recommends that such balance be approximately maintained.
3. DOE should increase travel fund allocations to allow program managers to attend scientific meetings both domestically and internationally. It is imperative that CESD program managers attend some of these meetings to enhance the impact of DOE sciences, exert leadership in setting research directions, and leverage DOE resources.
4. DOE should improve its electronic grant information system to better assist the program managers and support staff for program management.
5. Program managers should develop program-wide metrics of the performance and progress synthesis in addition to the quantitative measure of publications to measure programs and to enhance their impact.

The COV had individual recommendations for specific programs: ASR, ESM, and RGCM should maintain their proactive collaborations with the community and their investments in activities related to the Community Earth Systems (CES) Model. IAR should consider the establishment of aformal cooperative agreement with the Massachussetts Institute of Technology research team in meeting its objectives. TES should encourage other federal agencies to address how voids in ecosystem carbon cycle research at DOE, including both managed ecosystems and the oceans, can be filled and information about these elements of the Earth system be included in DOE modeling efforts. The Next-Generation Ecosystem Experiments (NGEE) has necessitated the adjustment of some SBR SFAs from geochemical processes to carbon-cycle research; SBR should maintain appropriate funding to retain key expertise in activities and radionuclide research. The Atmospheric Radiation Measurement (ARM) Climate Research Facility management was proactive in the development of the "best estimate" data sets; the program managers should continue these efforts. The Environmental Molecular Sciences Laboratory (EMSL) should continue to increase the user pool, especially to attract new investigators, including allowing postdoc researchers to serve as PIs of EMSL proposals. In recognition of the growing costs of instruments and maintenance for the CES the facilities, ARM Climate Research Facility and EMSL program managers should continue to engage the science community to set priorities and to maintain the proper balance of protecting the legacy data sets and acquiring new instruments.

In summary, the funding processes across all CESD programs are rigorous, appropriate, and well documented. The awards and projects are monitored effectively. The CESD programs are of high quality. They are nationally and internationally respected. The Program Managers are dedicated and effective. The COV made recommendations in the report on portfolio balances, travel, efficiency, metrics, CESM, program breadth, and usage and budget vigilance on facilities.

DISCUSSION

Stacey questioned the recommendation about postdocs principal investigators at EMSL and asked if proposals were rejected because they came from postdocs. Zhang replied that postdocs are not allowed to act as PIs. Baldocchi noted that postdocs are temporary employees, and institutions have to worry about continuity and responsibility. Zhang added that the situation is complex; the user facilities have different levels of engagement for different capabilities.

Stacey asked what had been discussed about the radionuclide research program. Zhang replied that it is important in many areas of research, and DOE has primary expertise and responsibility in that area. Therefore, the COV felt that it should be specifically emphasized.

Leung agreed with increasing the program managers' funds for travel. She asked whether there were any consideration of the National Science Foundation (NSF) in the discussion of potential symmetries and merging programs. Zhang replied that the NGEE is a program that could enjoy cross-agency support.

Penner asked what was behind the comment on system modeling. Zhang replied that it is difficult to organize these projects.

Ehleringer asked if there were a trajectory issue to be dealt with in Recommendation 2. Zhang responded that those numbers are steady; there were declines in FY10 and FY12.

Shaver stated that the growth of large programs that cross boundaries should be promoted to others, integrated with other programs, and jointly funded.

Randerson noted that, on page 56 of the COV report, there is a shift in the number of proposals. He asked why such a strong drop-off occurred. Zhang replied that the program focus narrowed as it matured. Thomassen explained that DOE was also transitioning to the SFA model. Money was not being taken out of the universities' allocation. There was a decrease in solicitations, also.

Penner said that there might be a case made for more coordination among the national laboratories.

Stacey commented that it is ironic that SFAs were supposed to provide more flexibility in funding and that the Committee is now hearing that they are restricting funding. Thomassen said that the SFAs are just completing their first funding cycle. The next set of reviews should be more meaningful in assessing this issue. Weatherwax added that the management at the laboratories is where the flexibility comes into play. Stacey said that, in Korea, program managers have to re-allocate 10% of their funding every year, wreaking havoc on some projects. Weatherwax pointed out that there are a number of SFAs doing different work on similar topics. Program managers must ensure that there is no duplication. There is a lot of pressure to get the most returns from all funds.

Robertson asked what the rationale was to move from competitive awards to collaborative research. Zhang said that it would depend on the history of the agreement. If the current arrangement works well, it would be continued. Thomassen added that cooperative agreements are still competitive grants that involve more input from DOE than a normal grant.

Merchant moved to strike the recommendation about postdocs as PIs at EMSL. Penner seconded the motion. The motion carried unanimously, and Stacey ordered that recommendation struck.

Stahl suggested that modelers of processes confer with large-model developers to find out what should be modeled. Wall added that researchers should also inquire about what type of data would make those models more robust.

Stacey asked if there were any other amendments to the report. Hearing none, he called for a motion to approve the amended report. Robertson moved, and Merchant seconded the motion; the motion carried unanimously.

A break for lunch was declared at 12:01 p.m.

Monday, October 28, 2013
Afternoon Session

The meeting was called back into session at 1:30 p.m. **Gary Geernaert** was asked to review the activities of the CESD.

Several positions are vacant, and a data informatics person (Jay Hnilo) has been added to the Division.

Three funding opportunity announcements (FOAs) have been issued so far in calendar year 2013. Preapplications are being solicited for four more in the coming year.

Reviews of the SFAs at Brookhaven National Laboratory (BNL) and Lawrence Berkeley National Laboratory (LBNL) were completed recently, with the BNL SFA being approved for renewal with minor changes and the LBNL SFA being approved for renewal. Reviews coming up in FY14 are the Lawrence

Livermore National Laboratory (LLNL) multilaboratory ESM SFA, the LBNL ASR SFA, the LBNL TES SFA, the PNNL multilaboratory ARM Facility), the SLAC SBR SFA, the Pacific Northwest National Laboratory (PNNL) SBR SFA, the ORNL multilaboratory RGCM SFA, the Los Alamos National Laboratory (LANL) RGCM SFA, and the PNNL EMSL Facility.

The meetings and workshops planned for FY14 are the ASR Working Groups on November 4–8, the Molecular Sciences Workshop on February 19–20, the Land-Use/Land-Cover Workshop on February 24–26, the Population Dynamics Workshop on February 27–28, the ASR PI meeting on March 10–12, the Regional Modeling Intercomparison Project in April, the TES/SBR PI meeting on May 6–7, the ESM/RGCM/Integrated Assessment (IA) PI meeting on May 12–15, and the Workshop on Mechanistic Models of Terrestrial Environments during the summer/fall of 2014.

The Community Earth System Model: A Framework for Collaborative Research was used in the IPCC program to develop a community model of the coupled Earth system: the atmosphere, ocean, land, sea ice, land ice, and terrestrial and marine biology.

At LLNL, a project on the human and natural influences on the changing structure of the atmosphere came out of IPCC'S Fifth Assessment Report (AR5). Its objectives were to compare modeled and observed patterns of the vertical structure of atmospheric temperature change, to determine whether an anthropogenic "fingerprint" is statistically identifiable in satellite observations, and to determine whether identification of a human-caused fingerprint is robust to current uncertainties in climate models and observations.

The decomposition of feedback contributions to polar warming amplification was studied to break out the individual process contributions to the polar-warming amplification. As the Arctic ice cover is decreased, dark areas are exposed; different types of clouds are produced; and different feedbacks are produced, in turn.

A subseasonal planetary wave pattern was investigated to gauge the probability of U.S. heat waves in terms of heat-wave intensities and distributions under future climate. The study identified a striking zonal wave number-5 Rossby-wave pattern that is responsible for many U.S. heat waves. Knowledge of this pattern can improve the model's probability forecasts of U.S. heat waves to 15 days in advance. This capability not only will improve weather forecasting but also will improve the understanding of future heat waves if wave number-5 events become more frequent.

A project that uses ARM data to investigate the dynamics of convection over the Sahel seeks to determine what triggers early monsoon deep convection. These convective features can propagate across the Atlantic Ocean and produce storms in the Caribbean and on the east coast of the United States.

A project on nonstatic nested climate modeling seeks to enable computationally feasible nonhydrostatic climate simulations with improved accuracy. These computations are highly data intensive and must have efficient algorithms. Nonhydrostatic simulations nested within reanalysis yield more-robust results. Further developments that have been suggested are super-parameterizations and variable-resolution nonhydrostatic modeling.

A new method simulates 3-D ice-crystal growth within clouds, a weakness of current climate models, especially for mixed-phase clouds. Ice-crystal-formation models must be more sophisticated. Growth rates are difficult to measure and model. This new model predicts evolution of crystal aspect ratio; growth rates along each axis are related to each other with parameters derived from laboratory studies of ice crystals.

A research project has discovered that mercury methylation is accomplished by novel micro-organisms from new environments. The research established a direct link between a specific gene and bacterial methylation ability. Bacteria capable of mercury methylation are more diverse than previously understood. This work provides an improved ability to quantify mercury methylation in a specific environment/location.

At EMSL, Alex Guenther now leads new Atmospheric/Aerosol Chemistry Science Theme; Tim Scheibe leads EMSL's Molecular Science Computing; and Scot Martin has been named to the EMSL Science Advisory Committee. Eight proposals were selected for the new EMSL–JGI collaboration; planning is under way for a 2014 call.

DISCUSSION

Robertson asked if this was the first round of SFA renewal reviews. Geernaert replied that, for some, it is the second round. Every SFA exploits the talent pool at a laboratory; they are under pressure, and they use different metrics that should be standardized. An effort is being made to adapt this approach to multi-laboratory SFAs. Robertson asked what metrics might be used for evaluating SFAs based on publications. Geernaert said that, very often, people report the number of publications but not where they are published. Some SFAs deliver code and cannot be measured against publication counts. Joachimiak noted that, on the issue of publications, some agencies require a digital object identifier (DOI) or other number that can be tracked. Baldocchi noted that a lot of projects produce data, not publications.

Mace asked what the vision was for AR6. Geernaert responded that the intent is to develop the appropriate analysis capacity to handle the Coupled Model Intercomparison Project Phase 6 (CMIP6) in support of AR6, determining where more models will be likely and where upgrades to the Earth System Grid Federation (ESGF) software infrastructure would be needed.

Randerson asked how one should assess CESD's declining numbers. Geernaert answered that what is desirable is to develop a major resource and figure out how many more resources are needed.

Todd Anderson was asked for an update on the Biological Systems Science Division (BSSD).

Since the last BERAC meeting, the annual Bioenergy Research Center reviews have been converted to online reviews because of the government shut down. The first of these online reviews went very well mechanically, although there are many areas for improvement. Coming up in December is the Small Business Innovation Research (SBIR) notice for taking Bioenergy Research Center translational science out to the workplace; the Genome Science Program PI Meeting on February 10–12 in Crystal City, Virginia; the biofuels SFA review, which will be tacked onto the end of the General Science Program PI Meeting; and the LBNL SFA review.

In FY14, two notices are expected for the Genomic Science Program and the Plant Feedstocks for Bioenergy Program. It is difficult to project funding resources because of the lack of a budget from Congress.

Seven new awards in plant feedstocks genomics for bioenergy have been made jointly with the U.S. Department of Agriculture (USDA). Ten new awards on systems biology enabled research on the role of microbial communities in carbon flux have been made. Computational biology is used in some of these projects with linkages to DOE Systems Biology Knowledge Base (KBase). Eight awards in carbon cycling and biofuels research have resulted from the joint call for exploratory collaborations. Some of these awards are leveraged by awards in genomics science.

Integration of actions by the BSSD and CESD is being investigated.

A Workshop on Research for Sustainable Bioenergy was held October 2–3, 2013, to understand the influence of biotic, abiotic, and genetic variables and combinations of variables on long-term plant-feedstock performance in the delivery of ecosystem services. A separate report on this workshop is being made at this meeting.

Key additions to the scientific functionality of KBase include metabolic and regulatory reconstructions for 5534 prokaryotic and 161 archaeal genomes, a phylogenetic framework for analyzing annotated metagenomes with species trees for taxonomic abundance, and a genotype-to-phenotype service that discovers genetic variations in plant populations and maps these to complex organismal traits. Different types of data sets are being added. Nearly 400 users have registered on KBase.us as a result of outreach activities. The application is still in command-line format; a graphic user interface will be rolled out next year.

The FY14 milestones of the DOE Bioenergy Research Centers are:

- The BioEnergy Science Center (BESC) at ORNL will continue to validate key genes in target consolidated bioprocessing microbes and enzymes and initiate modifications to achieve improved conversion and product synthesis; it will complete the sampling of poplar and switchgrass common gardens; and it will initiate testing of potential thermophilic microbes in biomass conversion.

- The Great Lakes Bioenergy Research Center (GLBRC) at the University of Wisconsin and Michigan State University will begin studies of cropping systems and land-use scenarios on marginal lands; begin translation of fundamental research on grasses to dedicated bioenergy crops; increase emphasis on next-generation fuels; and evaluate lignin valorization.
- The Joint BioEnergy Institute (JBEI) at LBNL will continue to validate function of genes for biomass traits in model plants and in biofuels production processes; develop tools that enable enzyme cocktail optimization for biomass deconstruction; and engineer central metabolism in target microbial hosts to facilitate fuels synthesis.

At the GLBRC, a new gene discovery clarifies the lignin biosynthesis pathway, identifying the enzymatic steps in lignin biosynthesis. One can modify the lignin pathways and make lignin more amenable to decomposition.

At the BESC, researchers have shown that pectin and xylan structures are covalently interconnected via arabinogalactan proteins. They are looking at pectins and proteins in the cell wall with the goal of producing new biofuels by modifying cell walls, making the cells more easily decomposed.

JBEI has genetically engineered yeast to produce higher yields of advanced biofuels. They have done this in *Escherichia coli*. Yeasts are more hardy for individual applications. Tailoring provided the highest recorded titers of advanced biofuels in yeast: 400 mg/L of free fatty acids, 100 mg/L of fatty alcohols, and 5 mg/L of fatty acid ethyl esters. There is still room for improvement.

In the Genomic Science Program, a method has been developed to fine-tune transcription and translation control in bacteria to accurately predict the expression levels of multiple genes introduced in engineered bacteria, producing a list of regulatory sequences that will allow precise genome engineering of bacteria for multiple purposes, such as the efficient production of biofuels.

In the Radiochemistry and Imaging Program, systemic acquired resistance has been investigated to use C-8, C-9, and C-10 dicarboxylic acids labeled with carbon-11 and carbon-14 to test the hypothesis that azelaic acid is mobile in plants, filling out the immune-response pathway that a plant follows.

In the Structural Biology Program, X-ray absorption spectroscopy (XAS) has shown details of solution structure to identify critical differences between solution and crystal electronic structures of a metalloprotein that helps explain its behavior *in vivo*. XAS was shown to provide valuable information for understanding the behavior of the active site of metalloproteins. Many systems being studied in BER's biological research involve such proteins, and this new capability will help enable progress in areas from biosystem design to biogeochemistry to carbon cycling.

Also in the Structural Biology Program, JGI has determined high-resolution structures of two cyanobacteria carboxysome proteins, starting from their synthesis. JGI researchers synthesized bacterial genes from *G. violaceus* and *T. elongatus* carboxysomes, enabling the expression, crystallization, and determination of crystal structures at Angstrom-scale resolution. Demonstration of the use of gene synthesis for structural characterization not only of the native protein but also of deliberately "designed" alterations vastly enhances functional analyses.

JGI has been very prolific, with 31 publications since the past BERAC meeting. It has also been a great facilitator to a number of communities.

DISCUSSION

Stahl asked Anderson to elaborate on what is going on in the Office. Anderson replied that there are researchers who want to integrate their research across program areas. A workshop was held to allow them to let the Office know how the research could be integrated.

Joachimiak asked how technology could be quickly applied to speeding up enzymes. Anderson responded that the centers are not being shy about applying that development.

Stacey noted that (1) KBase is widely known as a microbial database, and (2) the JGI and EMSL joint program should be expanded to a number of other laboratories. Anderson replied that the Office is interested in how facilities can be integrated. KBase has a lot of data on not only microbes but also plants and metagenomics. Merchant asked what plans there were to incorporate other genomes. Anderson responded that the flagship genomes of JGI will be included.

Robertson noted that DOE made many more awards then did the USDA in the joint feedstock genomics program. Anderson replied that it has not been an even partnership in terms of money. It is hoped that the cooperation with the USDA will be expanded in the future.

Zhao asked what the future plans (beyond their 10th year) were for the Bioenergy Research Centers (BRCs). Anderson answered that the budget projections for FY 15 will be coming up quickly, and the issue would be clearer then as discussions continued.

A break was declared at 2:52 p.m. The meeting was called back into session at 3:20 p.m.

Gary Stacey gave a BERAC member science talk and discussed innovative approaches to address global challenges in biological nitrogen fixation.

The prices for petroleum and the ammonium nitrate fertilizer derived from it have increased dramatically since the OPEC oil embargo of the 1970s. With the world population growing to 9 or 10 billion people by 2050, demand for nitrogen fertilizer could top 165 x 10^{12} tons per year. Because of inefficient uptake, a good deal of this fertilizer is entrained in runoff and produces algal blooms and other environmental and health issues in surface and coastal waters. Improving the nitrogen fixation by maize could lower the need for petroleum-derived fertilizer.

The Gates Foundation sponsored a meeting on enhancing biological nitrogen fixation in crop plants in April of 2012. It discussed developing a rhizobial symbiosis in cereals, introducing and encouraging interactions between diazotrophic bacteria and cereal crops, and designing a new organelle to fix nitrogen in crop plants. One funded project was engineering the symbiotic (Sym) pathway of cereals for recognition of nitrogen-fixing bacteria. This Sym pathway is a bacterium-infecting nodule that fixes nitrogen from the air. There is an evolutionary connection between endomycorrhiza fungal infection and such a rhizobium-induced nodule.

It is now known that several of the signaling steps are shared between the endomycorrhizal and rhizobial symbioses. From the fossil record, the endomycorrhizal symbiosis is seen to be very widespread and arose some 400,000 years ago; it is assumed that the mechanism rhizobial infection evolved from the endomycorrhizal symbiosis, which does occur in cereals.

Endomycorrhizae and rhizobia produce chemically related lipo-chitin oligosaccharide (LCO) signals, Myc-LCOs and nodule (Nod) factors. Many of the steps of the common pathway that produces nodulation and mycorrhization are already in the plants. One view is that a core set of symbiotic genes determines whether plants are capable of entering into a symbiosis with either rhizobia or mycorrhizae. There are two possible hypotheses to explain the lack of rhizobia symbiosis in some plants:

- They lack the ability to recognize the Sym signals (e.g., the Nod factor), and/or
- They lack the ability to couple this recognition to the symbiotic development pathways.

Research at the University of Missouri indicates that the second hypothesis is the correct one.

Pathogen/microbe-associated molecular patterns (PAMPS/MAMPS, small molecular motifs consistently found on pathogens) are recognized by pattern-recognition receptors (PRRs) in plants and animals, leading to the induction of innate immunity. Plants recognize these patterns and trigger signal transduction. Many microbe-associated molecular patterns trigger such plant defenses. The Missouri researchers studied one of these [flagellin (flg22)] in detail. Chito-oligomers involved in a synergistic effect with flg22 were identified. The Nod factor itself was found to reduce innate immunity [i.e., flg22 triggered the production of reactive oxygen species (ROS) in soybean leaves as measured by *in planta* bacterial growth]. It also worked in combination with other PAMPS and with other legumes; and the recognition of PAMPS occurred early. Adding in Nod factors induced the response, leading to a loss of flagellin-sensitive 2 kinase (FLS2):green fluorescent protein (GFP) on the plasmid membrane. This effect was also observed in corn and tomato plants. All plants have a receptor for chito-octaose, and the induction of plant defense pathways leads to the suppression of plant innate immunity and the induction of symbiotic development.

In regard to nitrogen fixation associated with grasses, colonization of grass roots by diazotrophic endophytes promotes growth. Inoculation of maize CD 304 with a commercial inoculum containing *Azospirillum brasilense* increases yield and drought resistance. There are reports in the literature of

significant levels of nitrogen fixation and incorporation into plants, but these reports are viewed with some skepticism by the wider scientific community, probably because the field is dominated by phenomenological reports with few mechanistic studies and even fewer molecular/genetic studies.

The Missouri researchers selected *Setaria viridis* (a problematic weed related to foxtail millet) as a model for the study of diazotrophic-plant interaction. *Setaria* produces a lot of seed and cycles quickly, is a C4 plant, is easily grown under greenhouse conditions, and has a recently sequenced genome.

To study the bacterial colonization, *Setaria viridis* seed was sterilized, germinated, inoculated, and planted. A number of parameters were analyzed (plant height, root weight, etc.). Of the first 30 genotypes of *Setaria viridis* screened, only 3 showed a significant growth response to bacterial inoculation. Therefore, it was concluded that plant genotype is a crucial factor. Inoculation of *Setaria viridis* A10-1 with *Herbaspirillum seropedicae* and *Azospirillum brasilense* increased weight and length. Roots colonized after 40 days of inoculation. Even with low nitrogen availability, NifH-Gus staining (where nifH is the marker gene that encodes nitrogenase reductase and Gus is β-glucuronidase) could be observed on *Setaria viridis* A10.1 growing under sterile conditions. Short-lived radioisotopes (C-11) were used to look at plant growth. Nitrogen limitation causes stress to the plant, resulting in changes in carbon metabolism. The presence of bacteria reestablishes normal carbon metabolism under nitrogen limitation. Not only uptake but also incorporation has been demonstrated. When nitrogen incorporation was investigated, a cumulative nitrogen-fixing rate of 125 ± 36 nmol per day was calculated from N-13 data. Approximately 30% of that nitrogen is acquired by the host and moved to aerial tissues, providing about 7% of the plant's total daily nitrogen requirement.

Conclusion - Increasing interest is being paid to biological nitrogen fixation, and the research record provides optimism that the research can be translated for practical benefit. Changes in the agricultural industry have created a more receptive environment for biological products. However, challenges remain, and agricultural research continues to be undervalued. University of Missouri research suggests that it is an inability to couple Nod-factor recognition to symbiotic developmental pathways that is the missing link in non-legumes, not an inability to recognize the Nod factor. It is believed that non-symbiotic, associative nitrogen fixation continues to hold significant promise, and research in this area will be stimulated by the adoption of *Setaria* as a model system.

DISCUSSION

Wall asked what the Rhizobium was in *Seteria*. Stacey replied that they are not a Rhizobium, they are an *Azospirillum*. Wall asked if they were inside the cell walls. Stacey said that they are intercellular, not intracellular. Sections are being taken with a confocal microscope to see the partitioning.

Robertson asked if they were inside or outside the plant. Stacey answered that *Azospirillum* is on the outside, and *Herbaspirillum* gets inside.

Joachimiak stated that nitrogen fixation is expensive for the host. If one relieves that tight regulation, one should be able to identify signatures associated with fixation. Stacey responded that some people are looking at the genome to pursue this question. What is desired is to develop a commercial corn variety.

Baldocchi asked whether the Nod factors' suppression of innate immunities would open up the opportunity for infection by pathogens. Stacey responded that Nod factors are short-term responses, so they do not expose the plans to pathogenic infections.

David Thomassen was introduced to discuss the BER responses to the BERAC Virtual Laboratory report.

The BERAC Virtual Laboratory report called upon BER to (1) capitalize on existing investments; (2) focus on the understanding and scaling of the fundamental biogeochemical, microbial, and plant processes; (3) measure elemental, energy, and water transfer across mineral, biological, and atmospheric interfaces; and (4) establish an instrument incubator.

The BERAC Virtual Laboratory report called upon BER to establish

1. Integrated field laboratories (IFLs) to identify opportunities for leveraging and extending BER investments to develop vertically integrated laboratories; strategically identify geographically dispersed

sites with the necessary subsurface, land surface, and atmospheric components; and develop instrument incubator programs

2. A Biosystems Frontier Network to integrate and expand technologies for microbial and plant physiology and phenomics to gain a better understanding of organism and community phenotypic expressions with complex and highly dynamic natural environments; the Network would include in situ and nondestructive "omics," quantitative measurement capabilities across expansive temporal (nanoseconds to years) and spatial (subnanometer to kilometer) scales in diverse environments, bioimaging innovations, and distributed research and instrumentation resources built on the core expertise of the JGI and EMSL
3. Cyberinfrastructure, Analytics, Simulation, Knowledge Discovery (CASK) to provide the computational infrastructure needed to integrate disparate and multiscale measurements, theory, and process understanding into predictive models, creating new knowledge for developing energy and environmental solutions; CASK would be built upon existing knowledge-discovery infrastructure (KBase and CDIAC) to link heterogeneous databases, develop multi-scale simulation frameworks and data-assimilation tools, develop advanced system-component models, and extend and link knowledge-discovery tools

BER scientific staff spent a day discussing this report and identified resources that could be used and gaps that need to be filled to address the goals of the report. In terms of the IFLs, the identified resources were ARM, NGEE, AmeriFlux, and field sites; the issues important to these resources that were identified as gaps were multi-cell organisms and climate, hydrologic processes, and global biodiversity and climate models.

In terms of the Biosystems Frontier Network, the identified resources were JGI, EMSL, the BRCs, omics research, and imaging research; the issues important to these resources that were identified as gaps were key timescales and interlinks among them, data types to integrate across scales, key boundaries between scales, key processes/means/variabilities, and critical interfaces between biotic and abiotic entities.

In terms of the CASK, the identified resources were KBase, CDIAC, the Program for Climate Model Diagnosis and Intercomparison (PCMDI), and modeling research; the issues important to these resources that were identified as gaps were challenges in data standards, metadata challenges, modeling at different scales, and climate–biology issues.

An internal BER seminar series (lunch-time, brown-bag seminars done in person and over the web) was put together on a series of modeling-related topics:

- From plant genomics to computation to climate
- Biogeochemical models across temporal and spatial scales
- Microbial genome-scale modeling
- Modeling the Earth
- Macromolecular modeling
- Climate-model construction
- Land modeling from watersheds to the globe
- Microbial-community modeling
- Atmospheric modeling from clouds to the global scale
- Plant metabolic modeling
- Integrated-assessment modeling

Other activities that the Office has undertaken in response to the report were to hire new BER staff to explore opportunities for data integration and modeling; to consider holding a future NGEE workshop to explore next steps (e.g., critical locations and ecosystems); and to consider what new strategies would be needed to pull diverse groups of scientists (from data collectors to modelers) together (e.g., jamboree space, visualization capabilities, and understanding NSF synthesis centers).

BERAC might be interested in organizing a workshop or set of workshops on visualization / phenotyping; if so, a charge to the Committee could be developed.

DISCUSSION

Stacey noted that these are not separate issues; the power is in the integration. Thomassen replied that that was the underlying theme of the whole day of discussion. Weatherwax added that there was a lot of cross-referencing of the parts of the report. Thomassen said that the elements developed to greater detail make the whole more robust.

Randerson noted that the NSF has a series of seminars, but there are a number of gaps related to climate that are important to BER. Thomassen replied that getting modelers and experimentalists together is difficult. Washington said that there are annual reports, workshops, and newsletters already. He worried about overload. Thomassen said that most of the programs have two-page descriptions, and they are not integrated. Stacey said that new kinds of tools are needed in biology. Biological research is centered on a small number of types of measurements. He encouraged that a workshop be held.

Joachimiak asked how one creates creative teams and stated that this workshop should be valuable in that regard.

The floor was opened to public comment. There being none, the meeting was adjourned for the day at 4:50 p.m.

Tuesday, October 29, 2013

The meeting was called back into session at 8:30 a.m. **Eddy Rubin** was asked to give an update on the implementation of the 10-year strategic plan of the JGI.

Two years ago, the JGI wrote a strategic plan in response to two publications that contained recommendations, the most important of which was for JGI to go from high-throughput sequencing to annotation with functional information. JGI had to bridge from biology and data sets to functional insights.

The JGI started the Emerging Technologies Opportunity Program to produce new capabilities; that program had 60 applications and 6 funded projects. One example is the Function-Driven Genomics Project, which uses Raman spectroscopy coupled with microfluidic isolation of targeted single cells to determine characteristics. Normally, one performed single-cell genomics by taking a sample, isolating a single cell, and performing a whole-genome amplification and genome sequencing. With function-driven genomics, functional analysis is done before doing the whole genome. There are several other similar projects.

The JGI–EMSL joint user program tries to synergistically link JGI and EMSL capabilities. A call produced 30 applications, and 8 proposals were approved. One of the successful proposals came from the University of Minnesota and the USDA on terpinoid biosynthesis in the fungus *Fusarium*. EMSL sorts out the organelles and then works out the proteomics and metabolomics; JGI does the genomics and transcriptomics to inform the proteomics and metabolomics.

Annotation of microbial genomes is the embarrassment of microbial geneticists. Geneticists have no clue what most of the genes whose sequences are generated actually do. This challenge needs to be taken on. JGI is using transposon-mediated mutagenesis–sequencing, in which the microbe of interest is subjected to transposon mutagenesis, is grown in media, and falls out of the population. The sample is then sequenced, and the lack of transposons identifies essential genes for the condition. This process is done hundreds of times for 50 conditions, and JGI is compiling a Functional Encyclopedia of Bacteria and Arachaea (FEBA) that allows large-scale annotation of microbial genes. This technique should decrease the number of unannotated genes. KBase is playing a big role in this process.

Another major challenge addressed by the strategic plan is state-of-the-art DNA sequencing. In the future, JGI will focus on specific targets, not commodity sequencing. The Pacific Biosystems (PacBio) DNA sequencer is a niche sequencer. It produces extremely long read lengths (average of 8,300 base pairs (up to 25,000 maximum) versus Illumina's 200) with an error rate of 16%. One reads the sample three times to get the right answer. The PacBio system also detects methylated bases. The technology current in 2002–2006 sequenced a genome with 49 contigs for $50,000 plus manual-finishing costs; today's technology sequences a genome with six contigs for $5,000 and no manual finishing costs. The new technology looks at the polymerase in real time, allowing the detection of methylation as the DNA is pulled

through. More than 200 bacterial DNA base-modification data sets have been completed and methylation patterns detected. The technology is really being pushed here.

The data generation of sequencing has increased tremendously, requiring high-performance computing infrastructure for the genomic big-data challenge. JGI has teamed with the National Energy Research Supercomputing Center (NERSC) to overcome the problems of data analysis and to drive down the costs for that analysis. The goal is to move appropriate JGI workflows to high-performance computing, such as all-against-all homology searches, development of a high-performance-computing metagenome assembly pipeline, and optimization of data-quality-control pipelines for high-performance computing.

Another challenge is to expand capacity to synthesize ("write") DNA to study genes and pathways and to manipulate genomes. It is desirable to synthesize the DNA, put it into an organism, and see what it does. JGI would like to provide this capability to its users, collecting these data and making them publicly available.

JGI has doubled its throughput to 4.0 million bases per year with the DOE BRCs the major users.

JGI also needs to encourage and support the organization and building of user communities around specific topics, such as those forming around plant microbial interactions. These activities are taking JGI beyond just commodity sequencing.

Prior to the DNA era, there were just two subsets of life, eukarya and bacteria. Carl Woese showed that there were more subsets, the biological dark matter. The genetic makeup of these archaea is not known. JGI is now going after the genomic sequences of all these branches of phyla, starting with the search for unexplored branches. It is also targeting its sequencing to dark-matter genomes. Earlier this year, a paper that provided insights into dark-matter genomes was published in *Nature* that will lead to reshaping the tree of life, the assigning of metagenomic data to an organism, and discoveries. With one project, JGI doubled the number of reads assigned to organisms, thereby revealing genetic potential. The Microbial Dark Matter Project expands the genomic representation of the tree of life and is a systematic step forward to an unbiased view of microbial evolution on our planet. Other branches are still being looked for.

It was found that codons (e.g., stop codons) can be recoded, which suggests that the canonical genetic code may not be all that is out there in the wild. Therefore, JGI looked at about 1,100 individual sampling sites and produced more than 15 terabases of metagenomic data and plus-phage data and looked for evidence of recoding. It looked specifically for the most radical and easy-to-detect conversion of a stop codon to an amino acid codon. The 15 terabases of unassembled sequence data were assembled into 450 gigabases of assembled contigs greater than 1 kilobase and put them through pipeline analysis. Expansion was looked for, and a lot of recoding was found. One could see where in the world this recoding occurs. These organisms can get into a host and recode that host's genome. It was found that, about 500 million years ago, this organism stopped using opal as a stop codon.

In summary, assumptions about the code are largely based on studies of cultured microbes. Metagenomics offers a broad, unbiased window into codon usage in nature. Overall, with the implementation of the strategic plan initiatives, the JGI is evolving as a genome science user facility to meet the scientific needs of energy and environmental research going forward. There is proof of this statement in the results of JGI's new programs and projects.

DISCUSSION

Joachimiak asked how one extends coverage for a single cell. Rubin replied that one can use much smaller volumes; one can grow things in micro-droplets; and there are other emerging technologies.

Stahl asked if there were any links with structural biology to move from structure to function. Rubin responded, yes; however, there is not a formal program. The JGI could team with EMSL to encourage researchers to produce the needed data sets.

Robertson asked how one identified these groups. Rubin answered that JGI has world-class researchers, and they go out into the community and recruit researchers to coalesce on a topic and submit proposals in response to the JGI's calls.

Baldocchi stated that the JGI's progress in assigning functionality is impressive.

Wall asked if JGI were getting thermophiles and psychrophiles in its dark matter. Rubin replied, yes, the processing conditions were such that these types of organisms would be detected.

Remington asked if DOE looks for people that are "outside the lamp-post light" to find new ways to attack the problems. Rubin replied that the whole universe is not being tapped. Weatherwax added that the problem is that one can get a lot of responses but that one does not have the staff to review that number of responses. Remington suggested that a self-reviewing, crowdsourcing approach may be the answer.

Stacey asked what the future of sequencing was. Rubin responded that JGI has a finite budget. In the future, sequencing will have a different role than it does now. The JGI–EMSL effort will remain open and produce new applications.

Stacey asked if the community were on the cusp of single-cell biology. Rubin said that it takes another company to produce the competition needed. The technologies need to mature to produce a commercial venture.

Scot Martin was introduced to give an update on Green Ocean Amazon (GOAmazon).

GOAmazon is looking for connections among the carbon cycle, cloud lifecycle, and aerosol lifecycle. The Earth is being changed rapidly and in many ways (e.g., in atmospheric methane concentration, carbon dioxide concentration, and ozone depletion); most of these changes have increased greatly in the past 50 years. In three systems, the rate of biodiversity loss, climate change, and human interference with the nitrogen cycle, the safe operating space has already been exceeded. For some planetary systems, there is not even an estimate on the effects being sustained. Most of the energy from solar radiation is deposited at the equator, and its redistribution is what drives the globe's weather. The greenhouse gases and particulates being put into the atmosphere upset the balance between insolation and outgoing terrestrial radiation. The Amazon also has a dynamic hydrologic system, but the uncertainties associated with its dynamics are quite big. Some of the forcing agents within that dynamic system are understood well, but some things have larger error bars than their observed values. This uncertainty results from the complexity of the system and the interaction and coupling of all the components.

The aerosol and cloud lifecycles are disturbed by anthropogenic changes. There are interactions between the biosphere and the atmosphere that affect the plant, atmosphere, hydrology, particle, and cloud lifecycles. Agricultural expansion and climate variability have become important agents of disturbance in the Amazon basin. There are some signs of a transition to a disturbance-dominated regime. These signs include changing energy and water cycles in the southern and eastern portions of the Amazon basin. The fear is that the Amazon may evolve from a tropical rain forest to a savanna; this has been projected by several models.

Amazonia is critical for water-vapor transport over South America. If the Amazon no longer contributes to this atmospheric water flow, southern South America would get less rain, which is critical to its agriculture. The Amazon basin has a strong coupling between the terrestrial ecosystem and the hydrologic cycle; the linkages among carbon cycle, aerosol lifecycle, and cloud lifecycle need to be understood and quantified. Currently, the susceptibility and expected reaction to stresses of global climate change as well as from pollution introduced by future regional economic development are not known or quantified.

The GOAmazon site is Manaus, a juncture of several rivers. It was a rubber-production center last century. In the 1960s, the military government decided to develop the Amazon basin. The population of Manaus has increased tremendously to 1.7 million people in 2009. Economic activity shifted from natural-resource extraction to resource processing and conversion to commercial products. So now Manaus is a large source of pollution. Data on meteorology is available back to 1850, allowing comparison of current conditions to baseline data. The vehicle fleet includes tractors, trucks, and buses that use diesel fuel and cars and motorbikes that use 60% gasoline and 40% ethanol. The Manaus power plant uses fuel oil but is transitioning to natural gas. There are relatively constant trade winds (east to west) that are typically 10 to 30 km/h at a 1-km altitude.

The research site's cloud cover is expected to be affected by pollution about 50% of the time. There are huge contrasts in carbon monoxide, particulates, etc. as the plume of pollution meanders, producing extremes from pristine atmosphere to heavy pollution. The biology of the forest partially controls the chemistry and physics of the atmosphere in Amazonia through the production of primary biological

aerosols, volatile organic compounds (VOCs), and biogenic salts. Salt and VOCs from the Atlantic Ocean and dust from Africa also contribute.

The chemistry of the regional atmosphere can be completely shifted under anthropogenic influences. The natural pathway goes away as the pollutants come to dominate the atmospheric chemistry. The lower updraft velocities of the Amazon basin make cloud-droplet number more sensitive to particle pollution. GOAmazon expects to gain insights into the atmospheric chemistry leading to improved modeling.

One hypothesis is that the Amazon forest will die back and turn into grassy plains. Studies of rainfall patterns have shown that a biome can shift with the intensity of the dry season. GOAmazon will produce data sets that will support models for projecting biome conditions and shifts.

The T-3 ARM Mobile Facility (AMF) will operate at the research site from January 1, 2014, until December 31, 2015, with radar, lidar, humidity measurement, etc. Aircraft operations will be carried out from February 15 to March 26, 2014, and from September 1 to October 10, 2014, thus covering both the wet and dry seasons. The aircraft operations will include cloud and atmospheric-chemistry probes and will coincide with the two intensive operating periods (IOPs) planned for the experiment. Criss-cross flight paths will analyze the plume characteristics, with two planes looking at altitude effects. Brazil and other countries will collaborate on this research. There is strong support from Brazilian organizations. A weather station has already been installed and fenced in.

The main research foci are the changing environment of Amazonia, the environmental sustainability and the sustainability of current terrestrial and aquatic production systems, and the variability and changes in climatic and hydrologic systems.

The site will operate for 2 years; mechanistic insights will be incorporated into models, and then model results will be tested against observations. Time series of aerosol optical depth at the Central and Southern Amazonia with MODIS [Moderate Resolution Imaging Spectroradiometer] and AERONET [AErosol RObotic NETwork] retrievals from 1999 to 2012 are already in hand. Models have become increasingly sophisticated, reflecting more couplings. GOAmazon will link these models to data sets produced by the research campaigns, focusing on chemistry and physics.

DISCUSSION

Stacey asked, with so many groups, whether there was an overarching management committee. Martin replied that he was the PI and that he had a steering committee with six foreign and four U.S. members. Aircraft are contracted through PNNL.

Robertson asked if there were any potential for mitigating crop effects by crop rotation or other techniques. Martin replied that the Amazon Basin is nitrogen limited. The emissions are very acidic. What this means for the basin will be looked at. Brazil has a world-class agricultural research capability. He did not know of any work on changing conditions from cropping. Robertson asked whether GOAmazon were doing anything on the crop systems in the 30% of the Amazon that had been deforested for crop production. Martin replied that this is a Central American project. The South American part was not funded.

Leung expressed an expectation that there are a lot of ice nuclei coming from biological sources in the Amazon. She asked what the opportunities were for studying these particles. Martin answered that the prevailing wisdom is that the Amazon cloud condensation nuclei are biological in nature (about 50%). It was proposed to investigate that bypath, but the topic was not funded.

Baldocchi asked how the growth and entrainment of particulates would be measured. Martin replied that lidar would be used, balloons would be launched every 6 hours, and aircraft sampling profiles would be taken to have closure on the model. Satellite data will allow upscaling. There are three satellite-data-interpreting staffers.

Mace asked what the relative importance was of ice form to warm-rain form. Martin responded that that is not well characterized. It is hoped to shed light on that issue. Mace asked if National Aeronautics and Space Administration (NASA) data show evidence of a Manaus plume. Martin answered, yes. The site represents three pixels in that data. The resolution of the satellite data is not great, but the effect of the Manaus plume is discernible. Mace said that the effects of the plume should be measurable up to 100 km downwind. He said that the large-scale difference in the meteorology is going to be different as the plume

wanders and asked how that difference will be accounted for. Martin replied that the team is aware of that issue and that some satellite data, instrumental data, and other sources of data will be used to address these limits.

Randerson asked if ozone input would be investigated. Martin said that that issue has been discussed. It is hoped that one of the ozone proposals will be approved.

Stacey asked if there would be any outreach to local schools and colleges. Martin responded that Brazil wants to improve its intellectual infrastructure. The President of Brazil launched a program to send Brazilian students abroad. Several of those students are being hosted in Harvard's laboratories, giving them a real educational benefit. There is a language barrier. Project staff members will interact with the local middle school.

Leung asked if anyone in the program was looking at mercury from mining and recycling. Martin replied, no. The closest investigation is on coal plant emissions. An independent project is looking at mercury pollution from mining and recycling.

A break was declared at 10:36 a.m.

The meeting was called back into session at 10:59 a.m., and **Catherine Ronning** was asked to report on the BER Workshop on Research for Sustainable Bioenergy.

The workshop addressed the use of marginal lands for energy-crop production and what environmental, hydrologic, and other effects may be produced by that land-use conversion. The goals of the workshop were to identify

1. Research gaps in understanding the interconnections between sustainable bioenergy feedstocks and ecosystem services, such as climate mitigation, water and nutrient conservation, biodiversity amenities, and pest regulation
2. Paths for developing models of plants, microbes, and environmental attributes that affect the sustainability of feedstock production and ecosystem services
3. Novel ways to link genomes and ecosystems with the tools of systems biology, genomics, and ecosystem science

Workshop participants came from a wide variety of institutions and expertise. There were observers from the offices of Energy Efficiency and Renewable Energy and Basic Energy Sciences. Plenary sessions were followed by breakout-group discussions oriented toward the three workshop goals. Discussions were summarized in a closing session.

Breakout Session 1 sought to identify the most compelling questions related to plant genome-phenome X environment interactions and their implications for sustainable bioenergy production and ecosystem services.

Breakout Session 2 sought to identify (1) ways in which 'omics and ecosystem knowledge can be linked to address gaps and opportunities and (2) research priorities for addressing gaps and opportunities. It was subdivided into discussions on

a. Sustainable biofuel crop improvement and environmental impacts
b. Below- and above-ground processes
c. Environmental effects and factors

Breakout Session 3 sought answers to the questions: How can one best utilize or adapt the tools of genomics to understand interactions and bridge molecular and ecosystem studies? What studies need to be done, and how should data be collected and managed? How can one ensure the delivery of ecosystem services while enhancing long-term performance of plant bioenergy feedstocks?

The workshop report is currently being written. The major themes of the discussions will be reflected in that report, including unforeseen consequences; ecoregional approaches; field trials; ecosystems' resilience to extreme environmental events and their recovery and adaptation mechanisms; modeling and scaling; soil organic matter decomposition and stabilization; biogeochemistry; when, where, and how spatial heterogeneity matters; the need for temporal studies that measure trends across gradients; plant breeding that maximizes ecosystem services; tradeoffs; plant-microbe-soil ecosystem interactions and

feedbacks; environmental inputs; long-term experiments replicated across environments and management practices; tying small-scale 'omics to the whole plant to the field; coordinated measurements, integrating data at multiple temporal and spatial scales; 'omics, computation; and imaging approaches to understand plant-microbial physiology and biogeochemistry.

DISCUSSION

Stacey asked when the report would come out and what its follow-up would be. Ronning replied that the first draft will be completed in a couple of weeks, and the report will be published by 2014.

Robertson noted that this was a good opportunity for researchers from diverse disciplines to compare notes and to propose concrete experiments.

Sally McFarlane was asked to report on the CESD Atmospheric Testbed Workshop.

The workshop was held August 5–6, 2013, at DOE Headquarters in Germantown, Md. Its goals were to improve coordination and identify potential synergies of the CESD atmospheric testbeds, improve linkages between testbeds and the ARM facility, identify ways to improve the utility of testbeds to the modeling community, identify gaps in the testbed portfolio, and develop a general architecture that would efficiently incorporate future testbeds. The participants were BER program managers, testbed representatives, ARM facility data product representatives, and model users.

Four BER atmospheric testbeds are in use today: Atmospheric Modeling (AMT) at PNNL, Fast Physics (FASTER) at BNL, Cloud-Associated Parameterizations (CAPT) at LLNL, and Climate Science for a Sustainable Energy Future (CESSEF) part of Earth System Modeling, a multi lab effort. Each of these testbeds is generally associated with a particular model, and they assemble data sets of field-campaign observations for use with that model. They employ suites of tools that graphically and statistically compare a wide range of observed and simulated quantities. The results of the testbed runs are used to identify errors in process representations in the model and to improve those representations.

The workshop was designed to assess what datasets exist, how they are formatted, what datasets are planned or needed, how their distribution might be better coordinated, and how ARM dataset development might be better coordinated.

The workshop identified distinctions and commonalities in model configurations, processes examined, and techniques. Areas identified for improved coordination include data sets and scripts for model initialization, expansion of testbeds to study land–atmosphere interactions, and analysis of aerosol indirect effects. Gaps that were identified include the need for standard formatting of datasets and documentation; user-friendly websites and quick-look plots; archives for model simulations; an ARM instrument-simulator package; data-assimilation methods and continuous large-eddy simulations (LES) to create a high-resolution reanalysis dataset over the ARM sites; and automation and availability to a wider community.

A workshop report is being prepared by the testbed and discussion leaders, a testbed session has been scheduled at the ASR Fall Working Group Meeting, a session on radar simulators is being scheduled at the ASR Working Group Meeting, a town hall on CESD testbeds is being scheduled at the American Geophysical Union meeting in December, and the idea of continuous LES simulations at ARM sites is being explored by an ARM/ASR/European Union collaboration.

Several efforts to enhance coordination have resulted from the workshop discussions: ARM translators will link testbeds and the ARM facility and will (1) discuss testbed-data-development activities and relate needs to ARM on Translator Conference calls and (2) facilitate movement of testbed datasets to the ARM PI data archive. The testbeds identified specific data and software to share among each other and with the wider community; datasets are currently being formatted and documented and will be hosted in the ARM PI archive or Earth System Grid Federation (ESGF). The testbeds identified potential joint activities, such as the coordinated study of aerosol indirect effect (AMT, FASTER, CAPT) and the test-case intercomparison activity from upcoming ARM field campaigns [e.g. GOAmazon and Marine ARM GPCI Investigation of Clouds (MAGIC)]. There is an ongoing DOE discussion on how best to coordinate these activities and align with programmatic goals.

DISCUSSION

Stacey asked Judith Curry if this addressed her concerns that she had expressed in a previous meeting about validating models with field data. Curry allowed that this is along the right lines.

Randerson stated that there would be a real value to a common single-column model results presentation for the different testbed campaigns.

Stacey opened the floor to Committee discussion. He called the Committee's attention to the new charge letter to conduct a COV of the Biological Systems Science Division. Stahl has agreed to chair that COV. Participation by other Committee members would be appreciated. In the past, the Committee has responded to BER staff requests. He asked whether there were other topics that the Committee wanted to address, such as the Virtual Laboratory report.

Stahl pointed to the problem of annotation, particularly of dark matter. There are orthogonal approaches among biochemistry, structural biology, and computational approaches that could address the biochemical products of gene screening and define function. Expertise within DOE could be coalesced to sort and discover new enzyme activities.

Joachimiak said that knowledge should be expanded through expanded annotation and through the assignment of functions to genes. This work is important for the future. There is also the issue of misannotation to be dealt with. The charge of KBase is to improve the annotations and transfer function onto those proteins. Stacey noted that many people are addressing computational approaches.

Stacey noted that a number of workshops have been held on annotation and stated that perhaps it is time to look at this topic again to get a view of the landscape and what the opportunities may be. Such a workshop should be in step with what JGI wants to do. Indeed, JGI could sponsor such a workshop. Remington commented that complementary approaches could leverage what JGI does. Joachimiak agreed that JGI would be the best institution to do it. He also raised the issue of promiscuity, which is important for synthetic biology and the creation of new pathways. These pathways need to be examined and defined. It is important to understand this issue at a mechanistic level.

Robertson said that the Committee has talked about a potential synthesis center; it may be time to host a workshop to discuss such a center. The Virtual Laboratory report encourages a more systems approach, but the Committee should also consider mega-sites to investigate the bedrock-to-clouds perspective. There are a lot of genotyping activities in industry centered on crop systems, and those activities are expanding to universities. A researcher at Texas A&M University has an instrumented tractor that he runs across a field to collect data. The community is limited in available instrumentation. There are a lot of opportunities to take phenotyping to a new level, into field cropping, ecosystems, and subsurface environments. A workshop is needed to connect biologists with instrument engineers and to identify the most appropriate systems etc. to investigate. Phenotyping came up a lot at the Workshop on Research for Sustainable Bioenergy. Ehleringer stated that the Jet Propulsion Laboratory has some such expertise. Remington commented that that is a great example of what can be accomplished if one gets the right people together.

Stacey pointed out that Monsanto found the computational capability to process, analyze, and display data that scientists can use. Remington pointed to the National Ecological Observatory Network (NEON) as a fertile source for environmental data.

Baldocchi pointed out that the community has lots more data than it used to. It would be good if DOE had a facility to manage these datasets so scientists could play with them.

Stahl commented that experts and instrumentation can do marvelous things.

Randerson pointed out that oceanography is another community that has been transformed by instrument development.

Stacey enumerated three themes that the committee seemed to be focusing on:

- gene annotation,
- synthesis centers, and
- visualization centers.

Baldocchi said that he did not know much about net energy. That might be considered in the future. Jacqueline Shanks had been submitted a comment by e-mail to the effect that agricultural and biosystems

engineers, electrical and computer engineers, chemists, materials scientists, computational experts, and standardization efforts along with biologists are needed to drive the questions that need to be solved.

The floor was opened for comment from the public. There being none, the meeting was adjourned at 12:01 p.m.