Biological and Environmental Research Advisory Committee (BERAC) Meeting November 2-3, 2017 Gaithersburg Marriott Washingtonian

BERAC Members Present
Gary Stacey, Chair
Judy Wall
Sarah Assmann
John Weyant
Dennis Baldocchi
Minghua Zhang
James Ehleringer
Huimin Zhao

Bruce Hungate

Anthony Janetos Designated Federal Officer

Andrzej Joachimiak Tristram West

Cheryl Kuske

L. Ruby Leung
Gerald Meehl
Geriad Meehl
Gerry Melillo (via telephone)
Gloria Muday
Guest Speakers
Celine Bonfils
Tim Donohue
Iav Keasling

Gloria Muday
Krista Jones Prather
Doug Kothe
James Randerson
Steve Long
Karin Remington
Jim Mather
G. Philip Robertson
Mary Maxon
Karen Schlauch
Daniel Segre
Gerald Tuskan

Others

Tiffani R. Conner, Science Writer

90 others were in attendance during the course of the two-day meeting and approximately 28 people viewed the webcast.

Thursday, November 2, 2017 Morning Session

BERAC Chair Gary Stacey called the meeting to order at 8.32 a.m. At his request, Committee members introduced themselves and provided updates on current research activities.

Following introductions and updates on current research activities, the meeting resumed with BER office updates, workshop briefs, reports, science presentations, and discussions. All presentations are posted to the BERAC website [https://science.energy.gov/ber/berac/meetings].

News from the Office of Science – Dr. Steve Binkley, Acting Director, Office of Science (SC) [Presentation posted]

Discussion

Addressing a question concerning the slow release of new funding opportunity announcements (FOA) and awarding of grants, Binkley said that the incoming administration instituted additional review steps for FOAs. He confirmed that the Early Career Research Program was one of the programs reviewed and that it is expected to move forward.

Maintaining U.S. preeminence in critical areas of science was a concern raised. Binkley stated that in his interactions with the Energy and Water Development Appropriations staff and the House Science Committee their view was one of uniform concern over the pace of progress internationally with respect to the U.S. There has been a lot of discussion in the current administration about the rate of progress in foreign countries in research areas of strategic importance. Despite statements of concern by Congressional staffers the overall share of U.S. investment in basic research has been slipping.

News from BER – Dr. Sharlene Weatherwax, Associate Director, Basic Energy Research (BER) [Presentation posted]

Discussion

Regarding the BER operating budget during the current continuing resolution (CR), Weatherwax said that the Chief Financial Officer indicates the budget number to plan to, which is typically the most conservative number. Because the House and Senate mark ups are quite disparate from that conservative number, BER has more flexibility and is operating closer to the FY17 budget for the CR period.

Weatherwax reminded BERAC that there is a learning curve and a shift in priorities in the beginning of every administration. Regarding FOA releases some accommodations have been made; for example, the period for the previous annual solicitation has been extended. Once FOAs are released, program managers will have a tighter time frame to complete the reviews.

Two rumors were voiced: first that the initial funding of the Bioscience Research Centers (BRC) will be lower than originally planned, and second that the Next-Generation Ecosystem Experiments (NGEE) Tropics program will have reduced funding or may be eliminated. Weatherwax explained that the BRC selections were announced and the awards are being finalized, but a CR is in place which limits the amount of funds that can be spent. Budget restrictions will cause the first year of the BRCs to be funded below the level expected. The BRCs are BER's priority and award supplements are anticipated up to the target amount, depending on the appropriation level. Regarding NGEE Tropics, the budget uncertainty has caused BER to give conservative guidance on future investments in NGEE Tropics.

A break was called at 10:14 a.m. and the meeting reconvened at 10:30 a.m.

News from Climate & Environmental Sciences Division (CESD) – Dr. Gary Geernaert [Presentation posted]

Discussion

Sea level rise, one of the interactions contributing to extreme weather events, is spread throughout the CESD strategic plan. One of the Energy Exascale Earth System Model (E3SM) project's big science challenges tied to sea level rise has to do with the future and evolution of ice sheet dynamics.

CESD supports data archives at Lawrence Livermore National Laboratory (LLNL) and at Lawrence Berkeley National Laboratory (LBNL). However, CESD's ability to utilize data from other areas is difficult because of interchangeable format challenges and the different resolutions seen in the models of the data sets.

Geernaert agreed with a BERAC member who mentioned turbokenetic energy and flux transference, saying that a problem is introduced when inferring the flux with dissipation techniques.

Neutron imaging of roots, in the drought context, has been completed at Oak Ridge National Laboratory (ORNL). The project, the first highlight to come out of the 2017 DOE SC Graduate Student Research (SCGSR) program, was a student fellowship award.

Geernaert indicated that once the approval process is complete, it is incumbent upon BER to execute and use the approved budget within the year. He said that the Regional & Global Climate Modeling (RGCM) + Earth System Modeling (ESM) and Atmospheric System Research (ASR) solicitations should be released once the budget passes.

News from Biological Systems Science Division (BSSD) – Dr. Todd Anderson [Presentation posted]

Discussion

KBase has made progress on reorganization since the previous review two years ago.

KBase suffered from an initial funding model that separated the computational component from the experimental component. Anderson explained that KBase was originally a science focus area (SFA) and in hindsight it was a mistake to call it that. From a BSSD point of view, the desire was to develop the framework rather than a specific computational tool.

Anderson indicated the biosystems design proposals are on a 5-year schedule. However, some of the concepts could be picked up by other, more frequent FOAs.

BSSD Committee of Visitors recommendations – Dr. Andrzej Joachimiak [Presentation posted]

Discussion

Joachimiak said the COV noticed scoring similarities in their extensive discussions concerning transparency in the decision-making process. Decisions should be documented in the records regardless of why a proposal was not accepted.

Joachimiak said that some SFAs are reviewed every year and are competitive while others submit an annual report. The BRCs have strong oversight because the same team of reviewers reviews all of the BRCs.

Weatherwax explained that program managers' travel and engagement in workshops is a budgetary pressure issue. Travel that is essential for safety takes priority and most of the program managers' travel falls outside of that category. Each program office in SC budget allocation for travel must be spread among all of the staff members.

The COV made the recommendation to link the Grand Challenges with the BER portfolio. With regard to the long-term vision and a balanced portfolio, the COV felt science is going to go forward no matter what and the ability of the program managers in BER to refocus and investigate new areas is essential.

The COV thought priority changes in KBase were due to internal evolution. The COV noted two main concerns: lack of descriptive publication on KBase and accessibility to the users. Stacey called a vote to accept the COV report. BERAC accepted the report unanimously.

The meeting was adjourned for lunch at 12:03 p.m.

Thursday, November 2, 2017 Afternoon Session

The meeting was called back into session at 1:15 p.m.

BERAC Science talk: Predicting Extreme Climate with Earth System Models: A Top-Down Look at the Southern Great Plains (SGP) – Dr. Minghua Zhang [Presentation posted]

Discussion

Zhang said people are working intensively to understand and model cloud aerosol microphysics and aerosol indirect effects.

The experiment was statistical rather than physical. This difference explains why adjusting the warming to the lower side would cause the precipitation to adjust up. Zhang speculated that the assumption – that precipitation should adjust down because the temperature difference between land and ocean would be reduced making the role of the jets weaker – would be accurate if the bias in the model were corrected.

The models missing strong precipitation events explained the relationship between temperature bias and future temperature change. The team averaged rainfall using the Atmospheric Radiation Measurement (ARM) sites frequency-intensity distribution of precipitation. Looking at the power of the increase of the precipitation distribution the team found the discrepancy. SGP is unique in making the results ungeneralizable due to the land-surface interaction and the frequent mesoscale systems.

Facility update: ARM – Dr. Jim Mather

[Presentation posted]

Discussion

Surface-water balance and improved parameterizations of turbulence in complex environments was mentioned. Soil-water balance is an area of increasing interest but shorter deployments make this collection somewhat problematic. ARM's best tool to study turbulence is the Doppler Lidar System but the deployments are driven by principal investigator proposals.

Mather remarked on sub-grid variability and sensible heat flux calculations, saying that before LES ARM Symbiotic Simulation and Observation (LASSO) implementation four boundary layer profiling sites were deployed to obtain turbulence measurements, and other measurements are being examined to augment LASSO.

Communication between ARM and KBase software engineers was a concern. Weatherwax reminded BERAC that ARM has a 25 year history and has clearly established systems for data management and archiving. KBase is newer and was not envisioned to be a database; rather a

framework for operating between datasets. The criticality of communication between software engineers was mentioned along with the need for BER to understand what is happening and how to facilitate connections between the scientists and engineers.

ARM management is being proactive in expanding interactions with the broader research community; their focus is on communications and awareness. The User Executive Committee will act as envoys to develop channels of communication with their communities and ARM will make better use of society meetings such as the LASSO Town Hall at the American Geophysical Union (AGU) fall meeting.

Early Career Science talks: Detection and Attribution of Regional Climate Change with a Focus on Precursors of Droughts – Dr. Celine Bonfils [Presentation posted]

Discussion

Bonfils had not looked at the droughts in Jordan, Syria, and Sudan which were suggested as potential fingerprints and proof of the models accuracy. She cautioned that while the models can provide latitudinal distribution of precipitation they cannot do it at the right location. Looking at particular regions is hard. Despite the fact that researchers have been able to attribute the California drought to human activity, they did not use the same techniques. It may be impossible to create a fingerprint of the California drought because there is too much noise.

A break was called at 3:05 p.m. and the meeting was reconvened at 3:15 p.m.

Introduction and talks from new Bioenergy Research Center Directors – Dr. Jay Keasling (Joint BioEnergy Institute, JBEI), Dr. Timothy Donohue (Great Lakes Biosciences Research Center, GLBRC), Dr. Stephen Long (Center for Advanced Biofuel and Bioproducts Innovation, CABBI), Dr. Gerald Tuskan (Center for Bioenergy Innovation, CBI) [Presentations posted]

Discussion

Lodging potential due to the altered mix of lignin and cellulose was mentioned. Tuskan said that the CBI, previously BioEnergy Science Center (BESC) at ORNL, evaluated lodging through the first 10 years of BESC looking at natural variation in both switchgrass and poplar. Lignin content varies from 15% to 32% in poplar trees. The trees examined at the low end (15%-16% lignin) were 90-years old and 1 meter in diameter having stood across droughts and wind-storms in the Pacific Northwest. The concept that low lignin causes lodging needs to be reevaluated. Long added that in sorghum the correlation between lignin and lodging is far from perfect and that CABBI feels they can deal with lodging within the sugar producing crops they investigate.

Long stated that water-use efficiency improvements have been shown at a modelling level. One of the results of rising CO_2 has been that C4 crops like sugar cane, sorghum, and maize are CO_2 saturated today, while at pre-industrial levels they were not. CO_2 saturation provides the opportunity to engineer a decrease in smart conductance.

Keasling said JBEI is considering techno-economic analysis (TEA), life-cycle assessment (LCA), and depletion of soils. If lignin is not considered, or if a larger fraction of the sugar content is not used, biofuels cannot compete with the oil industry. Scaling up the biofuels technologies will address the cost question.

Keasling stated that while the BRCs look similar there are large differences. For example, the BRCs are all looking at deconstruction but are using different deconstruction methods, the produced fuels are different, and the molecules each BRC is addressing are different. Over time the differences between the BRCs will become more apparent and the BRCs will evolve away from each other ensuring more ground is covered. While a 10-minute talk can leave the impression of similarities, each BRC only learned what was contained in the other BRC portfolios two weeks ago and are now discussing how to collaborate and optimize. There is no clear winner in the biofuels industry thus having all the BRCs testing the solution space to find the best strategies and solutions will move the industry forward. Tuskan relayed that the BRCs are talking about areas of collaboration, sustainability, TEA, and lignin conversion. Each of the BRCs previously developed certain capacities or abilities to characterize biomass or fuels and have a goal to collaborate more.

Donohue explained that gasoline is only 10% of the country's energy grid and 1/3 of the transportation fuels. Focusing only on improving gasoline is short-sighted therefore GLBRC is looking at all types of liquid fuels. The BRCs see bio-refineries operating much like petroleum refineries. Petroleum refineries make half of their money on fuels from 70% of the barrel and they make half of their money on chemicals from 20% of the barrel.

BERAC discussion of Grand Challenges Report – Dr. Gary Stacey

The Chair commended and thanked West for his efforts on the Grand Challenges Report and opened the floor for discussion.

The Chair accepted a request to use an earlier version of Figure 8.2 which represented multiscale cloud system coupling. Two versions of Table 7.1 were noted. West indicated similar inconsistencies were found and asked BERAC member to email him such things.

Verification of Table 7.1 capabilities indicators came from authorities from the User Facilities through the process of being sent out repeatedly for review by experts. The Executive Summary, which was reviewed and signed off on, is the last correct version. The Chair indicated the Executive Summary is a statement of conclusions.

A motion was made to change Grand Challenge 2.4 on p. xi to read "Understand the links between genotype and phenotype in single but very diverse organisms and in communities of organisms that interact in terrestrial ecosystems", striking "...to cycle carbon and nitrogen." Following a lengthy discussion the motion for the modification was seconded. BERAC members voted unanimously to accept the alteration.

The Chair asked BERAC members to discuss what they liked about the report. Compliments included a coherent, visionary report with actionable items, a separate facilities section, and an emerging technologies aspect.

Weatherwax explained that the process involves voting on the report, making final edits, posting the report to the website, and possibly having a limited print release. BER will review the report as a program and identify possible activities for action items. The Executive Summary was approved in the Summer and some of the items appear in the FY19 Budget Request.

More public attention was recommended for the Grand Challenges Report. Weatherwax reminded BERAC that the report answered a charge. Technically BERAC completes the report, votes on it, and issues a letter to the Director of SC in response to the charge. Weatherwax will make the suggestion of a broader public release to the Director of SC. Weatherwax stated that BER could generate a slide set for others in DOE to use when discussing the Grand Challenges Report.

Weatherwax explained that the NGEEs were envisioned to last 10 years and are not yet completed thus they will be continuing in some form into the period that the Grand Challenges Report covers. Weatherwax thought that alternative terms would be appropriate in the next versions of NGEEs.

The Chair clarified that the agreed upon changes were one edit on Grand Challenge 2.4, minor editorial changes for wording, use of an updated version of Figure 8.2, and a final review of Table 7.1. The Chair called the vote to accept the Grand Challenges Report with the identified edits. BERAC members voted unanimously to accept the report with the noted edits. The Chair asked that all edits be emailed to West by November 13th.

A BERAC member recognized Betty Mansfield and her team at ORNL for their efforts in helping with the Grand Challenges Report.

Discussion and Public Comment

The Biosciences Strategic Program Coordinator at LBNL read a statement, "Thank you for the opportunity to provide a public comment. The recent release of the BERAC Grand Challenges Report inspired a tremendous response at Berkeley Lab. We believe that these kinds of reports are influential within the Office of Science, but also greatly inform the national dialogue around biological and environmental research, including the philanthropic sector as well as the public sector. In fact, there was so much enthusiasm around the report that the lab hosted an internal visioning workshop on the grand challenges on October 16.

"77 staff from five scientific disciplines at the lab and of all career stages attended the workshop. Participants drove the selection of breakout group topics aligned with the grand challenges outlined by BERAC. These groups were: 1) user facilities, data standards, and data sharing, 2) carbon cycling and integrated environmental modeling, 3) high-throughput functional phenotyping, 4) efficient biological engineering in any host and production of biomaterials, and 5) microbiome prediction, design, and control.

"From the breakout groups, task forces are emerging to further refine the program concepts discussed at the workshop, and these groups are working on a suite of white papers that we plan to share in January 2018. We are looking forward to learning how others are inspired by the BERAC Grand Challenges Report. We welcome discussions with our other national lab and university partners, as well as any others with related interests, to brainstorm about the grand challenges BERAC has identified. Thank you for your insights and for the inspirational report."

BER staff members were thanked on behalf of the community for the outstanding job they have done under unusual circumstances in the last 12 months. The scientists in the community benefit from the talents and dedication represented on that staff.

The meeting was adjourned for the day at 4:46 p.m.

Friday, November 3, 2017

Weatherwax informed BERAC that Paul Dabbar's nomination for Under Secretary for Science had been confirmed by the full Senate late November 2, 2017.

Briefing: Exascale Computing – Dr. Doug Kothe, ORNL [Presentation posted]

Discussion

Electrical consumption and heat, GPUs in exascale, and the Chinese exascale chip were addressed. The Exascale Computing Initiative (ECI) is funding six U.S. vendors to address electrical consumption and heat. By 2021-2022 power on load will become more affordable even at 20-30 megawatts. Heat will continue to be a problem as form factor size is reduced, but there are creative ways to cool air with evaporative cooling and air cooling. Kothe referred to the GPU-side as accelerators. Great technologies are coming from NVIDIA and the ECI is interested in other accelerators by AMD, Intel, and IBM. ECI does not want to develop boutique codes that target a single architecture. China is moving aggressively; they have an indigenous chip and are running realistic applications. The Exascale Computing Project (ECP) is aware of what is going on in China, but is focused on developing their own capabilities.

Kothe used Trilinos as an illustration of progress on the standard software libraries being used in ECP. Trilinos is a go-to package with 100's of person-years investment. Trilinos is undergoing a complete overhaul to help the ECP teams hide the memory hierarchy complexity. While the application developers are getting used to relying on key technologies, a common question is what will happen when that team disappears. ECP requires a sustainability plan for technologies such as numerical libraries that must be stewarded at laboratories that are maintained well beyond ECP.

Briefing: Council on Competitiveness (COC) – Dr. Mary Maxon, LBNL [Presentation posted]

Discussion

Maxon was asked how BERAC could help with interagency coordination. The BERAC presentation provided an opportunity to think about the role of the COC in bringing together the agencies, industry stakeholders, and non-governmental organizations (NGO). COC can help drive the bioeconomy; BERAC could offer help to COC using their network of contacts.

Briefing: Interagency Working Group on Plant Genomics (IWGPG) – Dr. Cathy Ronning [Presentation posted]

Discussion

Funding of the plant breeding decision support tools is between the agencies and the organizations involved and maintenance of these may include subscriptions. IWGPG only coordinates activities among the different agencies and emphasizes the importance of the collaborations through the 5-year plans.

Ronning said that more education mission-directed agencies might be interested to partner with DOE to develop longer-term fellowship opportunities and pre-doctoral courses.

While holding joint investigator meetings in conjunction with the genomics-funded PI meetings had not been discussed Ronning stated most of the scientists IWGPG works with attend the International Plant and Animal Genome Conference (PAG).

IWGPG is thinking about inviting National Institute for Standards and Technology (NIST). Last year NIST held a workshop on standards for microbiomes in general and one for crop and plant microbiomes.

A break was called at 10:01 a.m. and the meeting was reconvened at 10:16 a.m.

Briefing: Interagency Microbiome Working Group (IMWG) – Dr. Angela Records, USAID [Presentation posted]

Discussion

The purpose of the IMWG Strategic Plan was to talk about what the Federal Government Agencies might plan to do. One topic had to do with data standards. The Department of Commerce is interested in data standards for microbiomes, but the degree to which agencies were targeting the Small Business Innovation and Research (SBIR) to support this industry was unknown. One BERAC member had seen many applications from small startups come through a SBIR panel on which she sits. Data standards were identified as one of the most important things for the microbiome industry and one BERAC member suggested that government should set the pace for establishing data standards. Another BERAC member said that genome sequencing committees have existed for at least two decades and need encouragement to continue.

Records indicated the IMWG Strategic Plan only lightly touched on the complications of data sharing. The U.S. government has an open access policy that could be a starting point on how to approach data sharing. Weatherwax added there is nothing in report that supersedes U.S. government policy on embargoes.

BERAC Open Discussion and Next Steps

BERAC has been given a new charge, to provide advice on the alignment among existing user facilities and research infrastructure to address current and future BER research challenges. Hungate will chair the subcommittee and he led the discussion. The new charge points to some of the opportunities and challenges identified in the Grand Challenges Report. Hungate asked BERAC members what the charge means to each of them.

The charge is an opportunity to look beyond current capabilities to future capabilities, for example cryo-electron microscopy (cryo-EM) has revolutionized structural biology yet that is not represented in any of the current user facilities. An exciting component of the charge is the openness to dream about what might be useful for BER science.

BERAC members thought that the phrase "optimal alignment" was an invitation to make recommendations on how a user facility could change to better serve future needs. There was agreement that the phrase "to develop new technologies" was wide-open, important, and allowed the subcommittee to dream a bit farther out than technology that is available but not widely used. The subcommittee was asked to consider a 10-year development period as part of the call.

Concern was voiced about the definition of a user facility. Questions arose if the term included software, databases, datasets, went beyond BER, or was restricted to national user facilities. Examples of user facilities included Joint Genome Institute (JGI), Environmental Molecular Sciences Laboratory EMSL, ARM, synchrotrons, beamlines, Nuclear Magnetic Resonance (NMR) facilities, cryo-EM, and computing. Other suggestions included AmeriFlux, field campaigns, partnerships with NASA, NIH, NSF, and user facilities with software components such as NWChemEx and MetaHipMer. One BERAC member requested a list of user facilities that are clearly defined by DOE to which the subcommittee could add. Referring to the definition of alignment, one person asked if systematic comparisons between user facilities had been conducted.

Beyond the definition of a user facility was the question of what "national community research infrastructure" meant. The Grand Challenges Report, 2nd action item in Chapter 5, states "create an energy sustainability modelling and synthesis center for multidisciplinary teams to address key energy-water-land research challenges". Hungate specified that the charge says "community research infrastructure" so the statement is definitely open for interpretation.

The role of training under component #3 in the charge was mentioned. Argonne National Lab allows researchers to send in a protein and work the machine remotely; EMSL will accept a sample, perform proteomics, and send the results back to the researcher. These two examples showcased optimization and a way to lower the inertia of entry into the user facilities.

Limiting the scope to the Grand Challenges was suggested as an organizing framework. The Grand Challenges has a number of infrastructure and user facility opportunities identified. One BERAC member suggested limiting the user facilities to only those that go beyond the individual operator and serve a larger number of investigators, possibly even spanning different agencies.

Some agencies, such as NSF, have relatively few facilities. BERAC was asked to consider what that means about the interaction with other agencies and non-DOE-supported research. Weatherwax mentioned the Memorandum of Understanding (MOU) between BER and Neon. The eXtreme Science and Engineering Discovery Environment (XSEDE) was recommended as a location to consider for DOE computational facilities.

Hungate mentioned the possibility of holding a workshop in Spring 2018. One person asked if the workshop could be held in conjunction with the Spring BERAC meeting. Weatherwax and West indicated that while exact dates would depend on other schedules, the suggestion could be considered.

Suggestions of first steps included naming volunteers during the BERAC meeting, receiving a list of user facilities to determine alignment with the Grand Challenges Report, and determining needed expertise to ensure adequate representations on the subcommittee. Hungate suggested using Table 7.1 in the Grand Challenges Report as a starting point, having subcommittee members represent the Grand Challenge areas and representatives from ARM, EMSL, and JGI attend a Spring workshop. Several BERAC members agreed that the subcommittee should have representatives from each Grand Challenge area. Another suggestion was to focus the scope on research that represents BER missions, along with the facility capabilities needed to support it.

The Chair reiterated that any other comments concerning the charge or offers to volunteer should be emailed Hungate. A BERAC member requested that all other members look at Grand Challenges Report before Nov. 10th to ensure everything appears as desired.

Three reports of interest to CESD were released by the U.S. Global Change Research Program on the afternoon of November 3, the final version of the Climate Science Special Report: Fourth National Climate Assessment (NCA4), Vol 1; the public comment and National Academies review version of all the chapters in the Fourth National Climate Assessment (NCA4) Vol. II; and the 2nd State of the Carbon Cycle Report (SOCCR).

Public comment

The Deputy Director for Biosciences at ORNL offered two comments. First, MetaHipMer is being integrated into KBase and the starting point for the integration of high performance computing capabilities into KBase. This should be available in the first quarter of 2018 and also there is close coordination between JGI and KBase on the adoption of this platform. Second was to point out that the Veterans Administration (VA) is starting to collect human microbiome and

epigenetics data for veterans in the Million Veterans database. The Deputy Director suggested that the VA, as well as scientists at ORNL such as Edmon Begoli who are working on this database should be included in the discussions. ORNL scientists have discovered common genes for disease pathology in poplar and humans and we need to ensure we can make these same kinds of cross species observations when we move to the microbiome.

The meeting was adjourned at 11:12 a.m.

Respectfully submitted, Tiffani R. Conner, PhD, PMP, AHIP