Biological and Environmental Research Advisory Committee (BERAC) Meeting

April 20-21, 2017 Gaithersburg Marriott Washingtonian

BERAC Members Present

Gary Stacey, Chair Sarah Assmann Dennis Baldocchi Amy Brunner James Ehleringer James Hack Andrzej Joachimiak Cheryl Kuske (via telephone) L. Ruby Leung Gerald Meehl Gloria Muday Krista Jones Prather David Randall Karin Remington Phil Robertson Karen Schlauch Daniel Segre (via telephone) David Stahl Judy Wall John Weyant Minghua Zhang Huimin Zhao

Guest Speakers Paul Adams Hans Christen John Dueber Dan Lubin Nigel Mouncey Stan Wullschleger

Designated Federal Officer

Tristram West

Others

Tiffani R. Conner, Science Writer About 80 others were in attendance during the course of the two-day meeting. About 17 people viewed the webcast.

Thursday, April 20, 2017 Morning Session

BERAC Chair Gary Stacey called the meeting to order at 9:02 a.m. At his request, BERAC members introduced themselves and provided updates on current research activities. [See presentations at https://science.energy/gov/ber/berac/meetings]

News from the Office of Science - Dr. Steve Binkley, Acting Director

Binkley expressed his appreciation for the BERAC members' commitment to the Office of Science (SC) and explained the importance of the Advisory Committees (AC) to the leadership of SC and DOE stating that they put a lot of stock in the advice from the ACs.

Rick Perry is the Secretary of Energy and Dan Brouillette, who has prior experience at DOE, has been nominated as the Deputy Secretary of Energy. However, there are no nominees or names for positions at the Under-Secretary and Director levels.

Congress will take up discussions of the FY17 budget upon their return to DC on Monday, April 25, 2017. There is hope they will pass an omnibus appropriation at that time. If not, there may be a short-term Continuing Resolution (CR) for 2 weeks for more negotiations, but if not, Binkley anticipates operating under a CR for the remainder of FY17.

The FY18 budget is currently being discussed. The FY18 budget blueprint in mid-March indicated a greater emphasis on defense and national security with a corresponding decrease in discretionary funds (i.e., research activities). The SC budget is proposed to decrease 17% (\$900M) which is the same as the FY08 funding level. SC has been working internally to accommodate the reduction. A formal proposal to Congress on the FY18 budget request will occur in mid-May.

There are approximately 40 out of roughly 140 political appointee positions that are filled within DOE; SC is still conducting briefings and meetings with the new administration to explain what SC does. The current focus at SC is the FY18 process and making progress on political appointees.

Discussion

Binkley was asked to share any priorities from the Secretary of Energy that effect Biological and Environment Research (BER). Secretary Perry has not mentioned anything directly related to BER, however, he has expressed being very supportive of the science mission and is aware of the historical role DOE has in science and plans to continue to support that. Secretary Perry has also made it clear that he intends to continue DOE's push on High Performance Computing (HPC).

News from BER - Dr. Sharlene Weatherwax, Associate Director

[Presentation posted]

Discussion

The BERAC Chair encouraged the creation of a slide on DNA synthesis that is similar to the slide on DNA sequencing. Some of the material in the presentation has been used in transition briefings and can be used and adapted to help communicate BER research.

The Chair recognized Dr. Weatherwax as a newly elected AAAS Fellow this year.

A break was called at 10:25 a.m. and the meeting was reconvened at 10:40 a.m.

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

Discussion

The blueprint for recalibrating Climate & Environmental Sciences Division (CESD) strategic plan with BERACs was discussed. BERAC has focused on the long-term vision/ plan, while CESD is focused on the shorter, 5-year plan to be adaptable, dynamic, and opportunistic. CESD realized that after 3 years the strategic plan is obsolete; that the strategic plan is not a fixed 5-year plan; rather it is adaptable and focuses on the highest impact opportunities.

From the solicitations slide, Geernaert indicated that 2017 Funding Opportunity Announcements (FOA) from CESD were issued in late 2016 and use FY17 money.

Regarding major gaps that are missing from the multi-scale approach, BERAC was assured that there is also a lot of coordination with other agencies. For example, concerning the oceans, CESD does not conduct oceans field work but relies upon data collected by other agencies. It was noted that oceans, a big component of earth system modeling, are not covered by other agencies right now. Geernaert said that National Oceanic and Atmospheric Agency (NOAA), Office of Naval Research (ONR), and National Science Foundation (NSF) have oceangoing ships within their budgets and those ships are collecting data. While the amount being collected may not be enough, CESD has to focus on where the most impact can be made.

Commenting on ocean data and illustrating a multi-agency and multi-national partnership, Geernaert mentioned that Argo floats have been deployed since early 2000s and have given the best observational picture of the global ocean in human history. Deep Argo floats are currently being developed which will sink deeper to sample the deep ocean.

Geernaert was asked about the importance of and responsibility for integrating human activity. CESD focuses on earth systems predictability and needs to incorporate every component that can possibly affect predictability.

News from Biological Systems Science Division (BSSD) – Dr. Todd Anderson

[Presentation posted]

Discussion

Anderson mentioned that the BSSD FOAs explicitly state they are not for renewals, but rather new projects. BSSD has expanded the FOA focus to go beyond biofuels to a range of bioproducts; the next iteration of the bioenergy research center program. The first iteration was planned for 10 years; expanding out to bioproducts makes sense and is a natural extension of what BSSD has been doing for the last 10 years. There are a lot more products possible and BSSD wants the body of knowledge that will result in more renewable sources of fuels and chemicals.

Anderson stated that one obvious challenge to KBase is creating a seamless collaboration between it and the Joint Genome Institute (JGI). Statistics on the current usage of KBase were requested and Anderson stated he could get the updated statistics to BERAC.

Using the illustration of blue carbon in coastal regions, Anderson was asked if there is a chance to interact with environmental part of BER and other agencies to study this recycling. In BSSD's main program, the focus is on terrestrial environments. The area where BSSD has had

more leeway to support marine systems is opportunities through Community Science Program (CSP) process at JGI, for example. BSSD has a relevant review of some of the more coastal areas and believes these are in scope primarily because of BSSD's interest in sediment processes and the terrestrial aquatic interfaces. Strictly marine work is discouraged unless there is a new demonstration of developing metagenomics techniques. It was pointed out that there is not a simple division between marine and terrestrial systems because some regions that are currently ocean/sea were lakes in the past. A lot of the microbial community work is done in marine or lake systems; the difference is it is studying systems in context. BSSD does study marine systems in context, but does not set out to study them specifically.

Response to CESD Committee of Visitors recommendations – Dr. Gary Geernaert [Presentation posted]

Discussion

The Chair indicated BERAC would return to the discussion of the COV report in the interest of time.

The meeting was adjourned for lunch at 12:33 p.m.

Thursday, April 20, 2017 Afternoon Session

The meeting was called back into session at 1:34 p.m.

BERAC Science presentation: Environmental and Hormonal Signals that Control Synthesis of Specialized Metabolites to Modulate Plant Development – Dr. Gloria Muday

Muday provided details on experiments and activities conducted with and by her laboratory group to understand the role of flavonols in root and root hair development, their relationship to guard cells and pollen viability. Using genetic mutations in mustard (*Arabidopsis*) and tomato plants, their work identified flavonol accumulation location and its modulation of Reactive Oxygen Species (ROS) levels related to plant growth, fertility and survival under environmental stress. Muday's findings include: quercetin and kaempferol are active flavonols; flavonol accumulation occurs primarily in root tips, guard cells and pollen. Flavonols modulate ROS to control signaling and development in root and root hair development, guard cell function, pollen viability and pollen tube growth. She concluded by sharing how her lab group's work is shaping K-12 students' understanding of plant physiology, genetic diversity, and genetically modified organisms.

Discussion

Muday was asked if the tt4 in Arabidopsis also shows infertility. In lab environments where the temperature is never above 23C, it has been shown to be perfectly fertile. Running the experiment under more stressful conditions is desired. Light also makes reactive oxygen species (ROS) and, in general, *Arabidopsis* do not survive under stressful conditions.

Muday was asked about data concerning the role of Flavonols and mechanosensing. She indicated she did not think mutants had been used to think about that.

Referring to increasing flavonol and heat resistance, Muday stated that they are currently testing the tomato and the purple tomato. In the tomato, Muday has one mutation that blocks flavonol conversion to anthocyanins that has higher levels of flavonol. Her lab is investigating the purple tomato's biochemistry and the hope is that it has a higher level of flavonols and a greater temperature response. Anecdotally, the only tomato left standing with fruit, still producing at the end of the season, is the purple tomato. This was a randomly isolated mutant and her lab is now crossing it into the common genetic varieties. The first order of business is to clean up the genetics of that mutant and put it in a context to be compared to a parent that has similar genetics. The hope is that more flavonols will help.

Muday was asked about the high levels of reactive oxygen species (ROS) and root hairs and if they are present as toxins or have a metabolic function. ROS can affect the structure of the cell wall, and perhaps they are affecting the cell wall to allow that rapid elongation that occurs in root hairs. In Muday's lab, they are considering what higher levels of ROS are doing, as well as trying to identify proteins that are oxidized in response to ROS.

With respect to the negative effects of flavonol, Muday said that in most parts of the plant flavonols are produced, but the levels go up and there are developmental controls. There is no anthocyanin in the roots; rather than anthocyanin, roots make the rest of the pathway and thus have higher levels of the flavonol, relatively speaking. Looking at a light microarray, the highest changes were in the enzymes and flavonol pathways; they are strongly regulated by light.

The Chair mentioned there are other reasons, besides heat protection, for purple tomatoes. For example, Cathie Martin has been using purple tomatoes in feeding experiments and has shown that they reduce cancer formation.

ARM Antarctica project – Dr. Dan Lubin, Scripps Institution

[Presentation posted]

Discussion

Lubin said that there have only been a few melt events like the January 2017 event since the beginning of the satellite record, but with increasing El Niño events more of these might happen. He did not know how representative their maps will be 10-50 years from now.

Lubin was asked if he was planning to include his radiosonde data in the reanalysis to see how much difference that made. Lubin stated that most of the data going to the reanalysis are from McMurdo, places in the peninsula, and those surrounding King George Island, but there is a big gap around West Antarctica. Lubin speculated that they may see some changes in the model output. The southern ocean is driving this melt event; they have the big picture, but there could be improvement. Lubin's group doubled the frequency from the sondes and other data at McMurdo, and he believes the weather forecasters for aviation there would be interested in it.

Lubin indicated that the melt was caused mostly by longwave cloud forcing. There is a cloud lensing effect that happens where the clouds are optically thinner than at mid-latitudes; it has been shown where the clouds transmit a lot of shortwave radiation but then also provide a thermal blanket. The surface turbulent fluctuations were fairly small, but they were mostly longwave clouds.

A break was called at 3:00 p.m. and the meeting was reconvened at 3:15 p.m.

Workshop Briefs: Exascale ASCR-BER Requirements Workshop and Advancing Cross-Cutting Ideas for Computational Climate Science (AXICCS) report – Drs. Dorothy Koch and Ramana Madupu

[Presentation posted]

Discussion

Koch and Madupu stated that one major challenge discussed in the AXICCS workshop was how much is possible to compute; there is a limit, a wall. The limitations of the next generation computers confirmed the confines to current computing capabilities, and there is a need for breakthrough computer technologies.

Koch and Madupu were asked about uncertainty quantification (UQ) and coupling. UQ and the challenge of working with big data were themes in the workshop; people who have tried to apply UQ methods to the earth system have found too many dimensions of uncertainty.

Center for Nanophase Materials Science: Technical Capabilities and Research Areas – Dr. Hans Christen, Oak Ridge National Laboratory

[Presentation posted]

Discussion

Christen indicated while there is a clearinghouse for a potential user to determine which of the five centers are appropriate for their research; most users call and are referred to the correct center.

Grand challenges for Biological and Environmental Research: A Long-Term Vision update and discussion – Dr. Gary Stacey

Several BERAC members shared preliminary ideas for grand challenges.

Eight grand challenges and seven action items were described, each in detail, for Earth Systems Research.

Four grand challenges and seven action items were shared by the Systems Biology group. It was suggested that the application or further development of synthetic biology is a challenge.

There were five overarching grand challenges in Microbial to Earth System Pathways, divided into three areas: microbial interactions structuring earth processes, trait-based approaches to scaling up, and microbial processes in earth system models. Shifting towards trait-based models was endorsed. Additionally, some mechanistic models looking at how plants and land use are changing over time are warranted. To get to finer scales will require mapping of disturbance and land use and improving data layers at higher resolutions as the models and machines get bigger and faster and the grids get smaller. For Earth System models, thoughts focus on plants and trait based modeling.

The weakest link was identified as annotating the genome in order to develop models. Distillation of that annotation would be to capture it in a trait-based format, identifying the key traits that allow resolution in the models. The ability to determine traits is only as good as the annotation. A concern was noted that there may be very critical traits, such as important molecules that are being produced, that cannot be assigned a trait simply because the annotation is not known. The microbial to earth system pathways group mentioned how central molecules and new analytical techniques are being employed.

There were five grand challenges and four actionable recommendations presented from the Energy Sustainability group. The speaker was asked if there is a framework, an infrastructure that could be used for an energy sustainability resource center.

One true grand challenge, five research recommendations, and four action items were offered by the Big Data & Computing group. A plea was made for the other writing groups to provide any feedback concerning data and computing. Data reduction was raised and alluded to in the presentation as the topic of keep/toss. The speaker's mixed feelings concerning data reduction were expressed.

The Emerging Technologies presenter shared information about unexpected things that happened since 2010, such as genome and metagenome annotation, advancement of single cell analysis and structural biology, and cryo-electron microscopy. The writing group's discussion topics and example of grand challenges were shared.

A description of the traditional role of facilities was stated. Facilities are important because a user facility does something that the user cannot do at scale or the user does not know how to approach. Facilities progress since 2010 included such things as light and neutron and molecular science facilities, nano-science centers, cryo-electron microscopy, and computational revolutions. Ten recommendations and six immediate action items were described.

Referring to missing or corrected data, the speaker offered two ideas: bridging hierarchies and creating knowledge from data.

Considering drones and instrumentation, working with NASA scientists at the Jet Propulsion Laboratory was suggested. The speaker indicated he used to collaborate with NASA scientists and stated that such collaborations are important.

Low-power, deployable, fast response, trace gas sensors were mentioned and the writing group discussed this as an issue.

Discussion

The BERAC Chair opened the floor to discuss all of the preliminary grand challenges presented.

A suggestion was made to pull common threads together rather than having each group write their reports separately. The Chair stated that when reading through the previous report documents, the common threads jumped out as obvious cross-cutting themes.

Writing the executive summary was addressed, including the need to include and prioritize common themes. While the cross-cuts would be important, there may be some weakest links in the chain in a particular area; thus, having each group submit a full report is essential.

There was concern about having standards to collect and add data to the database. The concern was deciding between junk and good data. Stories were exchanged among BERAC members of different examples of the effects of using junk data. Making a case for keeping the data, a BERAC member stated it was a matter of dealing with junk rather than tossing it all. An example of undiscovered information in junk data was the discovery of clustered regularly interspaced short palindromic repeats (CRISPRs).

A statement was made that working with the earth system model, which is approximately 14 orders-of-magnitude in time and space, yields the need for compelling big picture questions.

Returning to junk data, two points were highlighted and discussed. First was developing ontologies and standards, and second was deciding what is junk and dispelling it from the database. Junk is a very subjective term, but is separate from building standards and ontologies. Metadata that goes along with the experiment is extremely important and is the biggest grand

challenge universally. Often data processors have to simply clean data. Careful collection and annotation of data, including the provenance, would serve data processors well. ARM collects and saves all data, including raw data and quality-processed data; researchers can use the cleaned or raw data.

The Chair was asked when workshop participants from the working groups will be brought into the discussion of the report. The Chair offered a schedule to enable delivery of the Executive Summary and complete report by June 12: complete chapters are due May 8, report compiled and formatted by May 15, draft subsequently distributed for review, reviewers' comments are due the first week in June, and the final draft will be submitted June 12. Graphic artists will be available for the visuals, thus mock-up visuals should be sent with the May 8 draft. Additionally, copyrighted images should be sent to enable the necessary permissions to be obtained.

The publication date of the Exascale Requirements workshop report was requested. One of the authors indicated that it is only lacking a few images, and BERAC was assured that it will not be any problem to use that report.

Referring to the workshop participants' involvement, a clarification was sought and a suggestion made to involve them earlier, before the end of the editing process. The Chair indicated that he was open to ideas but did not think circulating an incomplete product was desired. He reiterated the constrained timeframe.

Discussion and Public Comment

Audience member noted a common theme mentioned in the meeting was data preservation which is a big deal in High Energy Physics (HEP). He stated it is not just about storing the data but also about ensuring the tools to access it are available. The Chair restated his point as "we might be able to learn something from other communities." The speaker agreed and added there are trade-offs. Big Data & Computing working group discussed that software processes and capabilities are able to progress through time.

The meeting was adjourned for the day at 5:43 p.m.

Friday, April 21, 2017 JGI facility update – Dr. Nigel Mouncey, Joint Genome Institute

[Presentation posted]

Discussion

The BERAC Chair welcomed Dr. Mouncey to his first BERAC meeting.

Dr. Mouncey was asked about JGI's perspective on the grand challenges. Mouncey said he would work with Chief Information Officer to provide something.

A question was raised about investigating unknown proteins and developing real phenotypes and activities for those. Mouncey has been having discussions with colleagues about imaging approaches that might allow the understanding of the function of unknown enzymes.

Mouncey agreed with the statement that in terms of sequencing, the true challenge is what is done with the sequences.

Mouncey was asked about his awareness of sensitives between user facilities and JGI and how he plans to balance those. He stated that JGI has opportunities to partner with other user facilities and that it is absolutely key to take advantage of the tremendous power house at the national labs.

Early Career science presentation: Repurposing the Yeast Peroxisome for Compartmentalizing Heterologous Pathways – Dr. John Dueber, UC-Berkeley [Presentation posted]

Discussion

Dueber was asked if he had any information on what causes peroxisomes to be so much bigger in some related organisms, if it is possible to use that information to make yeast grow larger peroxisomes, and if that would change some import parameters. Peroxisomes grow so large because they are methanol utilizers and they want to compartmentalize the oxidase reaction. An interesting question would be how to change the genetics of *Saccharomyces cerevisiae* to mimic that. That has been attempted on a small scale in single knock-outs and single over-expressions. The phenotypes usually are either larger with a reduced number of the peroxisomes or are smaller with a dramatic increase in the number of peroxisomes. The transport of proteins and metabolites are going to be affected by how many transporters are at the membrane and how much membrane is available. With better tools, we are interested in studying the whole suite of biogenesis genes under a screening pressure to see if larger peroxisomes are attainable.

Office of Science review of DOE lab LDRD – Dr. Karin Remington

[Presentation posted]

Discussion

The speaker was asked if the Lab Directed Research and Development (LDRD) is being used strategically to develop new capabilities or are labs simply picking the best science that is submitted. The labs visited use a mixed distribution of a top-down and bottom-up strategy.

A question was raised about multi-lab approaches, and if these are either encouraged or discouraged. Multi-lab approaches were neither encouraged nor discouraged. However, the current systems of management within the different labs may make such approaches more difficult.

LDRD was referred to as a tax and at what level that tax was levied. The tax is levied across the overall cost base at the laboratories. LDRD funding is congressionally mandated, but the discretion between the levels of 4% - 6% is balanced by lab management decisions. Universally, LDRD was thought to be a good value; none of the labs reviewed would want to do without LDRD. It is vital in order to develop new ideas and build the new workforce.

BERAC took a break at 10:00 a.m. and reconvened at 10:15 a.m.

NGEE Arctic project – Dr. Stan Wullschleger, Oak Ridge National Laboratory [Presentation posted]

Discussion

Wullschleger was asked about the carbon being released from the permafrost and how much is being recaptured. There was a range of uncertainty between 2010-2012; however, with

more work being done in Alaska, it is becoming apparent that there are more processes contributing to that simple question. Currently, CO_2 and methane can be measured, and there is some discussion about the net effect of vegetation regrowth and capture of some of the CO_2 . A lot of methane is still coming off of the systems because of the warming potential which is still troublesome from the modeling perspective.

Wullschleger was asked about the encouragement and facilitation of data sharing and communication with such a diverse group. He said a culture has to be established, an expectation must be set, and with time change takes place. The younger, early career staff and students are the drivers of the change.

Barrow has seven eddy covariance towers within 2 kilometers of the field site, and some interesting cross-site footprint analyses of that footprint and the flux is being done.

Data collected by Eugénie Euskirchen, University of Alaska, Fairbanks, is being used to develop synthetic data products for Antarctica and Alaska. However, not all of those data are in AmeriFlux or FluxNet. The team indicated Barrow had good facilities. In contrast, on the Seward Peninsula, the team has access to vehicles and has secured summer housing, but there is limited space.

Regarding existing challenges to make measurements over a pan-arctic environment and testing the model over a larger region, Wullschleger said they are getting started on that by developing international collaborations and looking for shared motivations and sets of measurements. The shared motivations and sets of measurements will ensure, from a model evaluation benchmarking standpoint, how to parameterize the models for pan-arctic simulations, and how to validate those and address issues of predictability and uncertainty.

Workshop Brief: Technologies for Characterizing Molecular and Cellular Systems Relevant to Bioenergy and Environment – Dr. Paul Adams, Lawrence Berkeley National Laboratory

[Presentation posted]

Discussion

Adams indicated that there was discussion about high-throughput, especially in biosystems design.

While the group tried not to make the meeting a grand challenges workshop, it was clear there are logistic challenges in terms of volumes of data, managing data, provision of data to community. From a scientific view, Adams thought the grand challenge was simulation of larger systems, but beyond that there are niche items, such as analysis for specific kinds of large volume data that require new math, and how to automate knowledge discovery from large data sets. Additionally, visualization technologies were identified as a challenge.

BERAC open discussion and next steps

The Chair opened the floor for general discussion among BERAC members. He reminded BERAC members of the opportunity to discuss the COV findings.

A more philosophical approach to the grand challenges was offered such as borrowing ideas from venture capitalists and the manner in which plants survive; set out a lot of seed and a few things will pop up that are unexpected. Expect the unexpected was the overarching mindset. LDRD allows something similar, having the ability to look for interesting ideas.

The amount of care BERAC should take to distinguish between a grand challenge and the next new research direction was mentioned. There are actually grand, grand challenges but there are also some things that just need to be done. Generally, BERAC would like to call out ideas that are indeed grand challenges, but also suggest some steps of how to get to accomplishment.

During the Race-to-Space and Cold War, there were overhead rates to do basic research because defense contractors told the military leaders that there were fundamental big gaps on DOE-side. LDRD is a good example of addressing similar situation; there will be some restrictions, but DOE is a mission agency.

A description of the difference between basic and applied research was offered: "all research can be considered like a bucket of water: some of us put in a thimble full, some of us put in a couple of gallons, but everybody is contributing to this bucket of water, and occasionally the water level gets to a certain height that we can actually tap it for something useful," by Earl Stadtman.

It was recommended that every few years the community asks what are the grand challenges and what new things are transformative. Because the future is unknown, at least we will be prepared.

A grand challenge is to use DNA sequencing to predict phonemics; to be able to understand information well enough to use it in a predictive manner. Non-destructive probing of soil cores was another grand challenge mentioned.

The Chair stressed getting a draft report to him by May 8th; it is very important to provide the BER leadership with community input to support programs and new directions.

A request was made to provide the writing committees with some direction on a reasonable number of actionable items. The preference was that the first draft includes everything that each group feels is appropriate in order to see which other groups made the same comment. Resonance becomes obvious from full reports because an item is expressed multiple times.

Public Comment:

No public comments were offered. The Chair adjourned the BERAC meeting at 11:36 a.m.

Respectfully submitted, Tiffani R. Conner, PhD, PMP, AHIP Science Writer Oak Ridge Institute for Science and Education, manage by Oak Ridge Associated Universities May 11, 2017