Biological and Environmental Research Advisory Committee (BERAC) Meeting Minutes April 25-26, 2018

Hilton Washington DC North/Gaithersburg 620 Perry Parkway, Gaithersburg, MD, 20877

BERAC Members Jerry Melillo
Present Patrick Reed

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Sarah Assmann Matthew Shupe

Katie Biteen David Stahl Designated Federal

James Ehleringer Kerstin Kleese van Dam **Officer**

Andrzej Joachimiak John Weyant Tristram West

Cheryl Kuske Huimin Zhao

L. Ruby Leung Gerald Meehl

Others

Maureen Leavitt, Science Writer

Approximately 90 others were in attendance during the course of the two-day meeting.

Wednesday, April 25, 2018 Morning Session

All presentations are posted to the BERAC internet site: https://science.energy/gov/ber/berac/meetings

BERAC Chair Gary Stacey called the meeting to order at 9:00 a.m. Eastern Time (ET). At his request, Committee members introduced themselves and provided updates on current research activities.

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

Discussion

The potential impact of the NIST (National Institute of Standards and Technology) 'Lab to Market' initiative on BER appropriations was discussed. Binkley stated that while there is a parallel effort within DOE led by Undersecretary of Energy for Science Paul Dabbar, there is no coupling of BER appropriations with the NIST initiative.

News from BER – Sharlene Weatherwax, Associate Director, Office of Biological & Environmental Research (BER)
[Presentation posted]

Discussion

After describing the budget process, discussion focused on information that might be available to better understand how Congress's budget will reconcile with the President's requested budget. Weatherwax explained that the Office of Science already met with Congress on the FY19 budget details. She stated the discussions were very positive and she believes Congress has an appreciation for long-term studies and the detrimental impact of reduced funding on these studies. She added at the time of this meeting, the House and Senate are in the process of marking up each other's requests with a goal to complete the effort by May. If the House and Senate cannot reconcile their budgets into one, it is likely that Congress will choose the lowest number from the House and Senate for each budget line and these will replace the President's request. Stacey acknowledged the significant and valuable effort of BER staff to communicate the value of their programs and maintain research program funding.

Addressing a question as to future environmental science research emphasis, Weatherwax provided the example of Congress increasing the Program for Climate Model Diagnosis (PCMDI) and Energy Exascale Earth System Model (E3SM) budgets from BER's request for FY18 when the spending caps were raised. She believes this action demonstrates Congress's commitment to environmental science research.

Further discussion focused on the impact of reorganizing the three modelling tracks. Weatherwax explained the primary value from the reorganization effort is minimization of the burden of accounting by management to tag budget lines. Most research activities will continue unchanged.

A break was called at 10:40 a.m. and the meeting reconvened at 10:53 a.m.

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

After the presentation, there was no further discussion by the committee.

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

Discussion

A general discussion focused on progress from workshops and highlighted the increased opportunities to couple biological science with environmental and earth system sciences. Geernaert commented that interdisciplinary collaboration is not new and has been informal within the Office of Science until recently. He attributed progress to efforts like the Interagency Strategic Plan for Microbiome Research. He also thanked BERAC for their very helpful comments provided in the Grand Challenges Report.

The meeting was adjourned for lunch at 12:00 p.m. ET.

Wednesday April 25, 2018 Afternoon Session

The meeting reconvened at 1:30 p.m. ET.

Response to BSSD Committee of Visitors Recommendations –Todd Anderson [Presentation posted]

Discussion

At the completion of the presentation, Stacey asked Joachimiak for comments as Chair of the Committee of Visitors. Joachimiak responded by saying the committee was happy with the overall process. He stated the committee appreciates BER's detailed responses and highlighting improvements.

With the completion of discussion, Stacey explained that each BERAC meeting includes a science presentation by one of its members. He introduced David Stahl as this year's presenter.

BERAC Science Presentation: Adding Biogeochemical Meaning to the Tree of Life - Dave Stahl (University of Washington) [Presentation posted]

Discussion

Discussion centered on the value of understanding microbial behavior in pure culture versus the environment in which it thrives. Stahl stated that he does imagine getting to a point where identification is possible without culture, but anchors are needed. A counterpoint to this statement was made that eukaryotes are identified without isolation. Additional discussion emphasized that archaea are common in deep sediment, are distributed all over the world, and are very important in carbon and phosphorus cycling. Therefore these organisms have a big impact on climate.

Stacey asked Weatherwax to introduce the next speaker. Weatherwax began with the statement that the challenge with data and computing is limited capacity to get the right information from the right data. To that end, she explained a framework was needed to accomplish this task. She introduced Deb Agarwal.

Data: ESS-DIVE (Environmental Systems Science Data Infrastructure for a Virtual Ecosystem) update, Deb Agarwal, Lead Principle Investigator, Lawrence Berkeley National Laboratory)
[Presentation posted]

Discussion

Agarwal answered a question regarding connectivity to KBase and Earth System Grid Federation (ESGF) by emphasizing the need for two-way data access, including KBase and ESGF. She further explained that external connectivity and cross queries are needed in real time to ensure users are getting the latest data. The difficulties in data formatting, such as those experienced by ESGF ten years ago, were acknowledged and Agarwal plans to visit Lawrence Livermore National Laboratory (LLNL) to discuss. She further mentioned she works with Ameriflux and developed a new standard for 300 PIs. While there were some complaints, the

extent of compliance is amazing. She attributed this success to involving working groups up front in the design process.

Regarding utilization of KBase tools within ESS-DIVE, Agarwal indicated it is not currently possible but that is planned. Agarwal further emphasized that this is not a research project. Her team is borrowing from everything they can find or access through KBase. Also, she intends to have a federated mechanism to preserve data in a curator role. This federation will allow for important cross-cutting research outside the Agency. She completed the discussion saying that digital library aspects will be an effort in collaboration with the Office of Scientific and Technical Information (OSTI).

A break was called at 3:04 p.m. and the meting reconvened at 3:23 p.m. ET.

Data: KBase Update - Adam Arkin, Principle Investigator, (LBNL) [Presentation posted]

Discussion

In response to a question on measuring co-expression and using the MAC biclustering model, Arkin explained that users can choose their own measurements using applications built by themselves or others; the knowledge engine would use all the data. Committee members stressed that the knowledge base is already sophisticated. However, there is a need for the users to become knowledgeable to use it effectively. The challenge is how to train the user so that "noise" is minimized. Arkin admitted it is a struggle and the team plans to work closely with "high-value" users that can train others. He suggested the best approach is to incorporate this material into undergraduate curricula.

A question was asked as to why the scale was defined so small (1m³). Arkin replied they chose that scope because that is where their expertise lies.

BERAC open discussion and update on Charge for Facility Evaluation and Alignment

Stacey asked Vice Chair Bruce Hungate to lead a discussion of the Subcommittee on User Facilities activities. Hungate indicated that the subcommittee convened to explore the scope of the charge, and has also reached out to Directors of facilities and working groups for input. The subcommittee has compiled responses that document contributions of facilities to grand challenge research questions and has begun to analyze and summarize this input. Their next step is to develop recommendations over the summer and deliver a draft report in time for the October meeting.

Discussion among BERAC members focused on non-respondents, or Directors who may not have recognized the priority for this effort in time to submit their response. Hungate stated they will continue to follow-up with non-respondents and emphasized that the subcommittee is open to additional input.

BERAC members were reminded that the Grand Challenges workshop was one year ago, before the Grand Challenges Report was published, and the committee should review the Grand Challenges to ensure that they remain relevant to steer their efforts. One example is Biosystems, which was not detailed in the Grand Challenges but is included in the scope of the BER research portfolio. The discussion closed with the acknowledgement of the good work completed.

Stacey invited the BERAC members to share any thoughts from the day. There were no further discussions from the committee.

Public Comment

Stacey asked for public comment and reminded commenters to identify themselves when speaking. Julie Mitchell (ORNL) commented that with respect to the computing grouping initiatives, she would like to see room for computational structural biology.

The meeting adjourned at 4:30.

Thursday April 26, 2018

The meeting was called back into session at 9:00 a.m. ET. Dr. Gary Geernaert introduced the Early Career Science Presenter, stating this is an important topic for the community and BER.

Early Career Science Presentation Adaptable Cloud Parameterization: An Early Career Project on Resolution Dependence – Bill Gustafson (PNNL) [Presentation posted]

Discussion

The discussion began with the question, "Is the confusion over weather versus climate a public perception problem?" Gustafson emphasized that climate models are optimized for different purposes and have different inputs. In addition, the scale of time is vastly different with weather working in days and weeks while climate works in decades. Asked if weather forecasts will improve with the increased resolution of climate models increases, Gustafson explained that although forecasts have improved with increased resolution, boundary and initial conditions as well as probabilities still represent a challenge on that scale. New mathematical methodologies are needed.

Additional inquiries as to the vertical structure of clouds and the parameterization impact on models were discussed. Gustafson emphasized the importance of layering and the understanding that different parameterizations need different things. He provided one example of aerosols. In current models, aerosols are input at uniform amounts. Layering can change that limitation.

The use of stochastics and exascale was discussed. It is difficult to get the data and computation to scale. This is where ensembles can assist. The National Center for Atmospheric Research (NCAR) model is an example of a large ensemble project. The forecasting community is using it more but large amounts of data are needed to tune stochastics.

Further discussion focused on what can be done with the Large-Eddy Symbiotic Simulation and Observation product (LASSO) to advance atmospheric research. Infrastructure is currently the priority. The spatial scale is not well-positioned, but Gustafson could offer no recommendations.

The next task will be parameterization of clouds to include an entire range rather than only shallow clouds. The Atmospheric Radiation Measurement (ARM) facilities offer different locations and cloud ranges; ARM sites to expand LASSO will be chosen within the next year. The additional resources and data are valuable, but integration will be an issue.

The BERAC committee concluded that the issue of scale is a challenge across many biological research areas. Examples of RNA 3-D structure and folding were mentioned as were spatial and temporal metabolism models.

Weatherwax introduced the next presentation, and indicated its importance relative to the new Office of Science budget. BER has not been working in Quantum Information Science, but their experience can be leveraged, particularly for improved sensors.

Workshop Briefing: Quantum Information Science – James Davenport (Basic Energy Sciences)

[Presentation posted]

Discussion

When asked about the potential for integrating probabilistic algorithms into quantum information science, Davenport explained that there are a limited range of opportunities. Machine Learning and Quantum Computing can incorporate probabilistic algorithms, but sensors and computing seem to be the most valuable applications. He emphasized that quantum science used to be philosophical and is only beginning to come to the fore. He expects opportunities in other areas will develop as the science matures. BERAC members discussed the United States' (US) standing in this realm, concluding that while China has a quantum satellite and Canada has quantum radar, the US does have a strong presence.

Answering a question regarding using quantum science to measure flux in and out of cells at nano-scale, Davenport stated that materials fluxes are not done, but magnetic and gravitational fluxes are. Currently it is possible to detect an image outside the cell, but further application is unknown. There is a need for probing with little or no invasion of conditions to better understand a cell's true state. Gustafson believes it can be done if the sensor stays coherent.

Regarding BER's plans to acquire quantum computers, Weatherwax explained that while BER is new to quantum science, it is included in BER imaging initiatives. If there are applications, BER can work on both algorithms and sensors.

E3SM Version 1 Release – Ruby Leung

[Presentation posted, video link: https://www.youtube.com/watch?v=8Df96rx3i9g]

Discussion

When asked about future projections of human populations and cropland or land use changes, Leung indicated these features are planned in version 2. She provided an example of how people may use energy, how that use will impact energy production, and how energy production will impact the environment.

Regarding weather prediction, Leung explained that this is an initial information challenge, and increasing resolution will improve prediction. She further explained that Earth System modeling is offering not just high resolution but also coupling which is important in long term simulations. High resolution can be used to test scenarios and perform numerical experiments.

BERAC Open Discussion and Next Steps

Stacey opened the meeting to discuss any further comments from BERAC members and reminded BERAC that it is very important for each member to be engaged in discussions during these meetings.

Public comment

No comments were provided.

The meeting adjourned at 11:11 a.m.

Respectfully submitted, Maureen Leavitt, ORISE May 14, 2018