Biological and Environmental Research Advisory Committee (BERAC) Meeting Minutes April 20-21, 2023

Bethesda North Marriott Hotel & Conference Center 5701 Marinelli Rd, Rockville, MD 20852

In-person attendance: BERAC, Invited Speakers, DOE Virtual attendance: Public

BERAC Members Present

Bruce Hungate, Chair	Maureen McCann	Asmeret Asefaw Berhe
Caroline Ajo-Franklin	Gerald Meehl	Ben Brown
Cris Argueso	Gloria Muday	Shreyas Cholia
Sarah Assmann	Dev Niyogi	Emiley Eloe-Fadrosh
Ana Barros	Himadri Pakrasi	Kjiersten Fagnan
Bruno Basso	Kristala Jones Prather	Forrest Hoffman
Sen Chiao	Patrick Reed	Mike Kuperberg
Leo Donner	Gemma Reguera	Devinn Lambert
Matthew Fields	Jeremy Schmutz	Giri Prakash
Robert Fischetti	Daniel Segrè	Ratna Saripalli
Jorge Gonzalez-Cruz	Karen Seto	Huimin Zhao
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Randi Johnson Matthew Shupe

Kerstin Kleese van Dam Designated Federal

Sonia Kreidenweis Guest Speakers Officer

Xiaohong Liu Adam Arkin Tristram West

Approximately 29 additional people were present on site, and approximately 248 were in attendance virtually during the course of the meeting.

All presentations are posted to the BERAC website: https://science.osti.gov/ber/berac/Meetings

Thursday, April 20, 2023

Introduction and BERAC Roundtable

BERAC Chair, Bruce Hungate, called the meeting to order at 9:00 a.m. Eastern Time and welcomed attendees. The science of nature and art go together; if the stories behind scientific research can be told more beautifully, more people will care.

BERAC Roundtable

Hungate invited all BERAC members to share BER-relevant thoughts. Discussion topics varied and included new centers, capabilities, tools, and discoveries while emphasizing the urgent need to leverage interdisciplinary, interagency, and international expertise and resources in the face of climate change. Research opportunities across scientific topics were shared and tied back to the need for a science enterprise that is diverse, equitable, and inclusive, as well as understandable to the public.

BERAC members emphasized the importance of libraries and rediscovering research from past decades as inspiration to advance their work. There was also curiosity around efforts to integrate new technologies such as artificial intelligence (AI) and machine learning (ML). Many were delighted to be able to meet in person.

New centers, initiatives, upgrades, and related efforts:

- The Climate Security Roundtable, convened by the National Academies of Sciences, Engineering, and Medicine (NASEM), is working to understand how climate change might affect national security. This includes climate impacts on migration, the livability of cities, and food security. Currently, there is no single federal agency that funds research in this area, despite its importance.
- The Center for Biofilm Engineering at Montana State University has used funding for new imaging instrumentation to acquire an inverted multiphoton hyperspectral confocal microscope and an upright digital lightsheet confocal microscope. The lab has also added a stimulated Raman scattering (SRS) module, which will allow stimulated Raman spectroscopy. These instruments will enable new quantitative biology and chemistry research to understand structure-function relationships at different scales.
- A new climate process team is focused on better understanding low marine stratocumulus clouds in the tropics. This collaboration is between the Geophysical Fluid Dynamics Laboratory (GFDL) at the National Oceanic and Atmospheric Administration's (NOAA) Office of Oceanic and Atmospheric Research (OAR) and the Nation Center for Atmospheric Research (NCAR). Approaches will involve large-eddy simulations and field campaign observations. This is a highly complex problem, and it appears the current field campaign methodology is inadequate; consequently, the team will be approaching DOE colleagues with expertise in the properties of these clouds with new questions.
- The Advanced Photon Source (APS) at ANL has suspended user operations in preparation for a yearlong comprehensive upgrade, which will increase the brightness of x-rays by up to 500 times. The upgrade will provide the ultimate x-ray imaging source and is relevant to BER in areas such as the rhizosphere and plant root uptake at nanometer resolutions and serial crystallography at high quality and rates. These changes will produce large data rates and volumes, so coupling with ANL's Aurora Exascale Supercomputer will allow for real-time data analysis.
- Howard University has established the Department of Earth, Environment, and Equity in an effort address the areas of climate change, climate resilience, diversity, equity, and inclusion (DEI), and workforce development. The first cohort will begin next academic year.
- The Materials Genome Initiative (MGI) is a federal multi-agency initiative for accelerating the deployment of advanced materials; BER should take this as inspiration to use plant genomics, systems biology, and synthetic biology to uncover design principles for better, more sustainable materials.
- Brookhaven National Laboratory (BNL) received funding from the Bio-preparedness Research Virtual Environment (BRaVE) program to research biosecurity using advanced computer modeling and epidemiology to understand how diseases spread, how to prevent that spread, and the effects of climate change in this area.

• The 2022 report from the BERAC Subcommittee on International Benchmarking has led to further conversations in biomanufacturing around global partnerships and how to partner with international colleagues to advance the deployment of biological solutions.

Notable appointments:

- There is a new Division Director for Global Climate Change at the National Institute of Food and Agriculture (NIFA) in the United States Department of Agriculture (USDA).
- The new Massachusetts Institute of Technology (MIT) president will be inaugurated on May 1 following a listening tour, where three major themes relevant to BER arose: students, faculty, and staff are united behind the urgency of addressing climate change; the importance of the life sciences to health and climate research; and the future of computing, especially around AI and ML

Discoveries and opportunities in modeling, plants, microbes, genomics, and urbanization:

- The climate dynamics of 600 years of major weather regimes in the Western United States (US) has been reconstructed. The data is from the Central Valley of California and is presented by watershed and irrigation district on a daily timescale. Multi-decadal events are highlighted; the recent family of atmospheric rivers that are ending the current drought show internal variability and uncertainty that compound the potential for climate change to transform these extremes.
- Data from the Atmospheric Radiation Measurement (ARM) User Facility and Atmospheric System Research (ASR) program are being used to constrain and improve climate models in light of the challenges around understanding cloud feedback.
- Research is investigating how the massive Australian wildfires from August 2019 to March 2020 might have affected the La Niña event which started in March 2020. Simulations show wildfire smoke was blown across the Pacific Ocean to the cloud regimes off South America; the smoke particles made the clouds brighter, causing less sunlight to reach the ocean and cooling the ocean surface temperatures. Carried by ocean currents and other processes, these cooler waters spread across the Tropical Pacific. Because of this, it appears that part of the inception of this La Niña event was externally forced. While the Australian wildfires ended in March 2020, feedback processes affecting ocean heat content persisted and sustained conditions for three years. This caused unusual atmospheric rivers in western North America that extended to Southern California.
- A virtual laboratory has been created to reproduce rainfall microphysics; microphysical
 processes will be simulated with the goal of cataloging data and determining whether
 fundamental questions have been asked correctly. In terms of cloud feedback, the virtual
 laboratory will allow the coupling of microphysics with large-eddy simulations to complement observational data.
- Research is determining how microbes get into the atmosphere, which microbes remain viable, their ecological impacts, and their impacts on cloud microphysics. Of special interest is biological ice nucleating particles and their sources. This work relies on the characterization abilities at the Environmental Molecular Sciences Laboratory (EMSL), a DOE user facility.
- Progress is being made to understand the connection between vulnerabilities in infrastructure and human impacts on natural environments, especially during extreme weather

- events such as Hurricane Maria. There is a special focus on how scientific research can guide actions to increase resiliency moving forward.
- The effects of urbanization on the sustainability of the planet are not well understood. There is no data available on the process level to understand how areas such as energy use, biodiversity loss, and habitat loss are connected. A new way of thinking must emerge to appreciate how cities are transforming biological and environmental systems.
- A study has been released discussing reflexive co-production as a framework to redesign roads to be equitable and green. This goal can be achieved through conversations among academic scientists, community groups, and the government.
- The National Getting to Neutral Report produced by the Lawrence Livermore National Laboratory (LLNL) is examining the greenhouse gas (GHG) emissions and carbon sequestration ability of bioenergy feedstock grown in the US. High-resolution models show the positive effects of perennials in reducing GHGs.
- The understanding of carbon use efficiency and its effects on ecosystem models is being revisited, including significant research conducted in 1960s. There is still much to learn in this area.
- The study of microbes will benefit from returning to historical research. Applying new techniques to pioneering studies will advance fundamental science and uncover ways microbes have adapted to a historically changing climate over history. Studies may be relevant to human adaptation to climate change.
- Research is being done regarding scaling microbial models. Some models are highly detailed, while others are simple, being represented by a single variable, so determining how to connect models of microbes of differing scales will be important moving forward.
- Progress is being made in phenomics and large phenotypic screenings; a significant book on the phenotypes of yeast was found that has not yet been digitized.
- There is increased attention around genetic engineering and clustered regularly interspaced short palindromic repeats (CRISPR) associated systems, especially in the use of complementary peptides on proteins to change gene function. These peptides accelerate translation in cells and can be added to plants by spraying the soil.
- Ideas in traditional protein and polymer chemistry can be applied to materials that are made by microorganisms. There are opportunities to leverage domain knowledge to accelerate efforts in this area.
- Genomics is seeing a dramatic increase in data collection thanks to new instruments. A ten-time increase in data collected is expected at a three- to five-times reduction in cost. These advances will be used to better understand what has happened in the past over evolutionary time and where natural systems will be going in the future.
- Genome-wide association studies (GWAS) are being used to identify correlations between genotype variation and climate adaptation in *Arabidopsis* and landraces of rice. For the latter, understanding what cultivars have been developed by farmers will help reveal selection traits; identifying these associations or correlations could help smallholder farmers adapt to climate change.

Discoveries and opportunities around AI and ML

 Process-based models and remote sensing imagery can provide feedback to understand soil health, especially when this data is linked with AI systems. Currently, there is not enough biological data for this research. However, advances in data collection from long-

- term systems will remedy gaps and provide information about impacts to soil from climate change and extreme events.
- A recent publication used deep learning and video gaming to create high-resolution data sets for climate models with the intention to create digital cities.
- There is a growing desire for communities to have local-scale climate information to create more resilient cities. This is the focus of work around Atmospheric Urban Digital Twins (AUDiT), on which several workshops have been held recently.
- Initial research to create an AI model for science has begun, using AlphaFold as a starting point. Efforts will bring in additional data to create a strong foundation for general biological sciences.
- The effects of AI/ML software such as AlphaFold and Rosetta are being seen in microbiology research. These tools are becoming highly utilized by students, so there is eagerness for how further developments in AI/ML and big data will advance biological knowledge.
- Research has allowed for the estimation of physically-based, hydrologically-constrained error structures in numerical weather prediction models. AI can predict the errors in these models, which is an important tool in the reduction of error structures moving forward.
- Large data sets are central to current scientific research; because so many people are involved in data generation, internal controls and standard processes are important.

Past and upcoming events

- Science from the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) expedition was presented at the 2nd MOSAiC Science Conference, held in February 2023. Highlights included research on atmospheric rivers; thermodynamics of sea ice and the competing dynamics in sea ice prediction; cloud and aerosol processes, including mixed-phase microphysics in clouds; freshwater melt and how it affects ecosystems; and biological and genomic research, especially in relation to physical systems. Presentations from early-career scientists were particularly impressive; presenters deftly communicated their cross-cutting research. Funding from DOE's ASR program helped many early-career scientists attend the conference.
- ANL held a poster session recently for high school students participating in the Exemplary Student Research Program, which allows students to use APS x-rays to study topics such as atmospheric aerosols and the uptake of chromium and lead in plant roots.
- The International Conference on Urban Climate (ICUC) will be hosted this year by the International Association for Urban Climate in Sydney, Australia.
- BNL will be hosting a digital twin workshop in October 2023.
- The Montana Biofilm Meeting in July 2023 will include a workshop on engineered living materials.

Call for an interdisciplinary, interagency, and international approach to socially translatable research that is diverse, equitable, and inclusive in practice and solutions:

- The importance of being able to make science relevant to the public and decisionmakers was stressed. BERAC members should consider how their research is presented.
- Members of the plant science community are participating in DEI training from the National Science Foundation's (NSF) Rooting Out Oppression Together and SHaring Our

Outcomes Transparently (ROOT & SHOOT) project. This program underscores the importance of diverse human perspectives in the scientific community and the need for a system that allows everyone to participate in research.

- There has been an explosion of multi-scale, multi-disciplinary biosecurity science recently, because of factors like the COVID-19 pandemic. Some of this work is being done through the National Virtual Biotechnology Laboratory (NVBL) and BRaVE.
- There is a need for larger scale efforts globally and a greater diversity of intellectual approaches in the climate modeling discipline, which will require a challenging balance; BERAC is central in advising how to move forward on these efforts.
- Scientists should consider collaborating with colleagues in South America and Africa, who have traditionally been left out.
- The hard work at the DOE on the recent Energy Earthshots Initiative call was applauded for its ability to break barriers across disciplines and offices.

DOE Introductory Remarks – Dr. Asmeret Asefaw Berhe, DOE SC Director

Berhe thanked BERAC members for their guidance of the SC. BER-funded science continues to serve the public. Highlights include the first climate model run on an exascale computer, the launch of the ARM Eastern Pacific Cloud Aerosol Precipitation Experiment (EPCAPE) in February 2023, and the creation of the National Virtual Climate Laboratory (NVCL).

Congress has recognized the critical role of the SC through the authorization of \$50B over five years from the Bipartisan Infrastructure Law (BIL). If approved, the FY24 budget will be \$8.8B, which will allow SC user facilities to be funded at approximately 90% of their rebaselined operations. Broadening the participation and retention of individuals from underrepresented groups remains an FY24 priority, with funding supporting Reaching a New Energy Sciences Workforce (RENEW) traineeship, Urban Integrated Field Labs (IFLs), and Climate Resilience Centers (CRCs) at Historically Black Colleges and Universities (HBCUs), Minority Serving Institutions (MSIs), and emerging research institutions.

The Energy Earthshots Initiative is designed to drive integrated program development across the entire DOE, utilizing leading science and technology innovations to address the technological challenges and cost hurdles that hinder important climate solutions. BER plays an important role in advancing the basic science that underpins these initiatives.

The SC continues to address recommendations from the BERAC Subcommittee on International Benchmarking report, which will be used as a baseline to measure future progress. Berhe also looks forward to the results of BERAC's charge on a more unified data framework.

Low-dose radiation research was part of the BER portfolio until 2016; because of renewed interest from Congress, SC is requesting FY24 funds for reinvigorated efforts in this area. As a result, BERAC was asked to provide input on the potential scope of an impactful low-dose radiation research program in BER, including what complementary research efforts might be undertaken with other federal research agencies.

Mentioned previously, broadening participation and retention of underrepresented groups is a major SC priority. Direct stipend levels of SC-supported graduate fellowships have been set at \$45K annually and all solicitations communicate that graduate students should be paid a living wage. SC is encouraging all funding applicants to review their internal policies and procedures to achieve the goal of paying graduate students, trainees, and post-doctoral fellows a living wage. Other efforts include expanding RENEW traineeship opportunities to all SC programs and nearly

doubling program funding in 2023; the Funding for Accelerated, Inclusive Research (FAIR) initiative to build research capacity infrastructure and expertise at institutions that have been historically underrepresent and minoritized in the SC funding portfolio; and Promoting Inclusive and Equitable Research (PIER) Plans, which require applicants to describe how their research or conference proposals will contribute to DEI.

Publicly funded scientists have a responsibility to communicate their work to policymakers and the public. Berhe encouraged attendees to share their research findings with the community and educate the public about the value of science.

Discussion

An individual asked about training resources that the SC might be able to provide scientists for sharing their research with the public and with decisionmakers. **Berhe** stressed the importance of taking the time to learn new communication skills and suggested seeking out communication professionals at national laboratories and universities for training resources. There are also resources and opportunities available through Office of Communications and Public Affairs (OCPA) within the SC.

A BERAC member mentioned the importance of providing living wages for graduate and postdoctoral students and asked whether SC is well positioned from a budget perspective to adjust grants accordingly. **Berhe** mentioned this requires prioritizing SC resources, and increasing graduate student pay is a high priority. Without a living wage, many graduate students cannot participate or focus on their research. The SC has control over SC-supported fellowships and can only provide guidance to universities, with the hopes that this will help stimulate conversations on this topic on local and federal levels.

News from the Office of Biological and Environmental Research (BER) – Dr. Gary Geernaert, Acting Associate Director

[Presentation posted]

Discussion

Clarification was sought around the Urban IFLs and AI; will models look beyond state estimation and examine complex adaptive human-earth interactions? **Geernaert** confirmed this; the Urban IFLs are intended to create a paradigm shift in the study of predictability. At least three Urban IFLs will use digital twins with the intent to develop simulations incorporating ML. Teams are encouraged to be novel and creative to push the envelope in using these capabilities.

An individual sought an explanation of what Critical Decision 0 (CD-0) and Critical Decision 1 (CD-1) mean. **Geernaert** explained CD-0 is a summary document to initiate the project that contains consensus on the mission need and why DOE should develop it. CD-1 offers funding and budgeting specifics.

Excitement was expressed over ARM's cloud chamber research efforts, and information was requested about its location and operation. **Geernaer**t explained that a cloud chamber was a high priority for atmospheric science, and BER sees it as an important investment for future collaboration with other agencies. More information will be presented by McFarlane.

A BERAC member asked about the role of BSSD at ARM and the Urban IFLs. **Geernaert** confirmed that BSSD is not playing a role in the Urban IFLs. BER is looking at ways to bring the divisions together, but does not see the Urban IFLs as a strong candidate to do that.

There was an inquiry about additional workshops around the fundamental science drivers for the Energy Earthshots Initiative and how BERAC members can be ambassadors for it. **Geernaert** remarked dedicated workshops are not planned but may be considered. The current charges are the top priority for BERAC members, so it will be determined what contributions can be made around this initiative.

An attendee was curious whether there have been discussions to expand the Urban IFLs to smaller urban corridors in the US or to partner with urban areas in the Global South. **Geernaert** said BER will initially stick with the current four Urban IFLs and consider expanding later. The selection criteria for Urban IFLs were whether an urban region had a diversity of communities regardless of size. Internationally, BER has been discussing with the World Meteorological Organization (WMO) about connecting to their urban programs. Sister cities are also being considered to broaden international coordination and collaboration.

A BERAC member suggested creating a clear strategy for expanding the Urban IFLs and asked whether there can be planning grants ahead of large funding initiatives to level the playing field. **Geernaert** appreciated the suggestion and will take it up internally at BER.

The role of BER in supporting efforts around grid modernization and energy infrastructure was questioned. **Geernaert** mentioned BER has had discussions with the DOE Office of Electricity (OE) about predictive modeling with their grid modeling. This discussion led to the hiring of a climate resilience manager at BER, emphasizing the connections that have been made between the basic sciences and applied sciences.

Hungate dismissed the meeting for lunch at 12:15 p.m. and reconvened at 1:30 p.m.

Update on Earth and Environmental Systems Science Division (EESSD) – Dr. Sally McFarlane, Acting Division Director
[Presentation posted]

Discussion

An inquirer wanted to know how to get climate research information included in the NVCL portal. **McFarlane** remarked the NVCL team is currently reaching out to the national laboratories and suggested getting in touch if the data is not there once it is launched in May 2023.

A BERAC member sought more information on ARM's cloud chamber research. **McFarlane** stated the NSF-funded cloud chamber at Michigan Technological University is not large enough to produce precipitation, so BER is taking the first steps of developing a mission statement about what creating a chamber large enough to produce precipitation would look like.

Information on the US-European Union (EU) Modeling of Transition Pathways Working Group was requested. **Geernaert** has been working with the Joint Research Centre (JRC) in Seville, Spain to create a collaborative, bilateral approach for transitional pathways to carbon neutrality. The next step is a one-day session at Snowmass Summer Meeting in June 2023 to create a roadmap.

An individual wanted to know how BERAC can get involved in the presented initiatives. **McFarlane** mentioned breakout sessions at primary investigator (PI) meetings. Through the discussions at BERAC meetings, input can be given on the highest priorities and how to move these efforts forward.

Update on Biological Systems Science Division (BSSD) – Dr. Todd Anderson, Division Director

[Presentation posted]

Discussion

Questions were held for the final discussion period of the day.

United States Global Change Research Program (USGCRP) Decadal 2022-2031 Strategic Plan – Dr. Mike Kuperberg, Executive Director [Presentation posted]

Discussion

An attendee asked about the fourth pillar in the strategic plan ("Collaborating Internationally"); why does the current budget have no contributions from the Department of State or United States Agency for International Development (USAID)? **Kuperberg** explained these agencies are consumers of data in order to understand climate risks, but they are not investing in global change research.

A BERAC member questioned who will provide the interface between the science and the stakeholders; many are looking towards private sources, but it is unknown whether that information can be trusted. **Kuperberg** agreed and hoped one day there will be an integrated, comprehensive climate services program in the US, but in the meantime, it is up to the research enterprise.

It was wondered whether the "engaging the nation" aspect of this initiative involves the Department of Education. **Kuperberg** said the Department of Education is not part of the USGCRP; the emphasis is on coordinating research and not education, although the need for education was acknowledged.

An inquisitor asked whether there is a need for a communications aspect for the USGCRP, as it will broaden the stakeholders involved. **Geernaert** interjected and mentioned a communications workshop on climate change last year; the lessons learned will be brought into upcoming PI meetings.

The engagement with indigenous knowledge during the process was appreciated; will that be transferred over to the CRCs and working with MSIs? **Geernaert** could not answer this question, as each of the applications for the CRCs were quite different.

An individual was intrigued by the mention of tipping points under Pillar 1; what is being done to understand those tipping points and the readiness to absorb shocks driven by climate change? **Kuperberg** understands tipping points over a geologic time perspective; USGCRP does worry about them and is working to understand what should be done. The socioeconomic aspects are important but the vast majority of USGCRP's funding is for the natural sciences.

National Nature Assessment – Dr. Mike Kuperberg, Executive Director, USGCRP [Presentation posted]

Discussion

Curiosity was expressed about the level of engagement with young people that has occurred around this program. **Kuperberg** stated the engagement has been broad, although more

targeted outreach to youth can be done. Most communication has been with underserved and indigenous communities. MSIs and tribal universities have been notified of the request for information (RFI).

A BERAC member wondered about the connections between the National Climate Assessment (NCA) and the National Nature Assessment (NNA) and whether there are lessons learned from the NCA. **Kuperberg** affirmed these connections, but work is being done so the NNA is not forced into the NCA model and format. The NNA would like to build on the NCA, especially the ecology chapter.

Appreciation was expressed for thinking about the NNA in an outside-the-box format, as many will not take the time to read these materials as a document; it is time well spent to think through formats other than reports. **Kuperberg** pointed out that the NCA had an art competition and a poem from the US Poet Laureate. The team behind the NNA are open to creative thinking.

An attendee asked how BERAC can contribute to the effort from the view of future research. **Kuperberg** was open to suggestions and stated BER research has long supported efforts like the NNA.

Hungate dismissed the meeting for a break at 3:26 p.m. and reconvened at 3:37 p.m.

Energy Earthshots Initiative – Ms. Devinn Lambert, Deputy Director of Crosscuts and Energy Shots, Office of the Under Secretary for Science and Innovation

[Presentation posted]

Discussion

The Energy Earthshots team was congratulated for the project, but the winner-takes-all funding approach was questioned as it shuts out some communities. **Lambert** agreed there are alternatives to single large investments using mechanisms such as funding opportunity announcements (FOAs), Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) funding, and user facilities to address the gaps.

A BERAC member wondered about the exclusion of solar power from the initiative. **Lambert** stated solar technology is at a place of broad deployment and the Energy Earthshots are looking to target technologies that have large inequities in fundamental science. In terms of renewable energy, enhanced geothermal and floating offshore wind were identified as areas where critical gaps might occur without this investment.

Urban Integrated Field Laboratories – Dr. Jennifer Arrigo, Environmental Systems Science Program Manager, EESSD

[Presentation posted]

Discussion

An individual commented on the potential for Urban IFLs to be models elsewhere and suggested preparing to take a leadership role. The ability to bring together different stakeholders was commended. **Arrigo** said this was a testament to the teams that have considerable history in building strong community coalitions.

The possibility of deploying ARM measurements sites to Urban IFLs was asked about. **Arrigo** mentioned Urban IFLs can apply to the current call for ARM Mobile Facility proposals.

Curiosity was expressed about how Urban IFLs can be translated globally. **Arrigo** said the Southeast Texas IFL (SETx-IFL) is specifically documenting the process of launching the laboratory, which will be able to determine the scalability of IFLs.

Workshop Briefing: Artificial Intelligence/Machine Learning for BioEnergy Research (AMBER) – Dr. Huimin Zhao, UIUC

[Presentation posted]

Discussion

A BERAC member wondered whether ML might help improve access to information in libraries that is relevant to research. **Zhao** mentioned how Chat Generative Pre-trained Transformer (ChatGPT) is often wrong and does not include scientific literature in training. This might be a chance for DOE to take the lead in building a large-scale language model for bioenergy research, which can help form hypotheses and make more precise predictions.

More information about hybrid models was desired; these combine knowledge we already have with ML. **Zhao** recognized the need for hybrid models in the biophysical area and sees the value of combining physical models with ML for greater precision. **Kleese van Dam** interjected about two approaches for hybrid models; using mechanistic models to train the AI and using AI to speed up a mechanistic model.

An individual remarked about scales where accessing data is difficult; how do you democratize that data? **Zhao** said ChatGPT has not solved that problem. **Kleese van Dam** mentioned approaches like privacy-preserving AI and federated AI, where the model is trained on a private data set but does not expose information publicly. Another approach is where access to data sets also includes the compute facilities to analyze that data.

The idea of establishing data banks and building specific models on top of each was met with approval. Are there divisions between traditional ML and deep neural networks (DNNs), random forests, and support vector machines? **Zhao** discussed this division during the process and emphasized the use of deeper learning tools, which are very powerful in research applications.

Interest was voiced about the process of advancing technology so AI models can discern between public and private data. **Kleese van Dam** sympathized with this challenge as the models lose data identifiers once they are trained. It is much easier to use public data sets that have identifiers. **Zhao** added the possibility of leveraging pretrained language models for deep learning. **Hungate** remarked this would be helpful for reproducibility.

An attendee asked about research around genetic algorithms that can look for equations that describe a system; is this still being done? **Kleese van Dam** has not seen this recently, but there are natural language processing models that can extract concepts out of existing literature.

BERAC Discussion

Hungate shared the low-dose radiation SC charge letter. What would such a program look like in BER? A response to this charge will be due to SC in one year in report format.

Reports about ionizing radiation creating soundwaves in cells were referenced; this type of radiation can affect the polymerization of cytoskeleton proteins, potentially affecting gene expression and downstream biological processes. There are also many unknowns around how low doses of radiation affect uranium-reducing bacteria. Lastly, there is curiosity around how climate

change will affect the dose of ionizing radiation both human and biological systems will be exposed to. **Hungate** liked these suggestions, as BER has a lot to offer in the model systems research area.

A BERAC member wondered whether the charge is specific to humans or can apply to all organisms. Anderson provided some background in response to this; DOE is home to a lot of the foundations of nuclear medicine, and there has been a long presence on the technology side of human health. Low Dose Radiation was formerly in the program portfolio, which was an extension of DOE's history in radiation biology. The low-dose area was focused on doses below 100 millisieverts (mSv), in which there is a significant amount of uncertainty on human health effects. Anderson clarified that an exposure between 5,000 and 7,000 mSv is lethal, and the global background radiation level is ~3 mSv; it is approximately double that in the US because of access to medical device imaging. Epidemiological studies to date have not been able to resolve to sufficient detail or certainty whether low-dose radiation causes cancer or other health effects. BER was involved in research from a systems biological approach that can lend itself to more detailed studies in animal models, but there are always transition issues from artificial models to humans. BERAC has looked at this charge before, and BER will provide information on that previous report, along with a strategic plan on the topic from the National Academy of Sciences (NAS). There is also a recent interagency collaborative report from those who either have existing low-dose radiation programs or radiation biology programs.

An explanation was sought about DOE's reasoning and the timing for this charge. **Anderson** explained the previous Low Dose Radiation and Nuclear Medicine programs were ended in 2016 to move the BER portfolio towards bioenergy and environmental science. Since then, there has been a concerted effort from Congress to bring the Low Dose Radiation program back.

It was presumed high energy beams and low-dose radiation have similar physics, but long-term reactions are different. There is a lot of understanding on how x-rays interact with materials and tissue, but not how tissue recovers from that interaction.

An individual mentioned BER expertise in understanding genomes and their changes. The Joint Genome Institute (JGI) has developed single-cell sequencing capabilities; but it is unclear whether these capabilities can be applied here. It might be fruitful to see the effects of lowdose radiation on microbiomes, which in turn affect humans. In response, a BERAC member added single cell research falls under the National Institutes of Health (NIH), but BER can look at technology development, nuclear DNA, and reproductive DNA from plant and microbial perspectives. BER capabilities can be used to collaborate with NIH on the human development side. It was agreed the NIH would be a good partner, but Veterans Affairs (VA) might be better. They have homogenous, well-collected data sets from following patients for long periods of time. There are existing collaborations between the VA and DOE. Another attendee noted the potential to collaborate with the National Institute of Environmental Health Sciences (NIEHS) around occupational exposure and the National Aeronautics and Space Administration (NASA) around radiation exposure to astronauts. Anderson added fruitful conversations have occurred with the National Cancer Institute (NCI) and the Advanced Scientific Computing Research (ASCR) program. There were strong connections with NASA during the previous Low Dose Radiation program, although space radiation is often different and higher energy. NASA has an existing radiation biology program.

Areas where BER can provide complementary input without overlapping with others were considered; the DOE is unique in having national laboratories that are equipped to measure

radiation. The Defense Advanced Research Projects Agency (DARPA) is another organization interested in space radiation.

The relevance of BER's capabilities around metabolism and isotope tracing was discussed. Rare events at the atomic level and quantum chemistry calculations might also be pertinent.

A BERAC member is already looking at radon exposure in urban areas, which might tie into the Urban IFLs.

The growing interest in identifying somatic mutations around cancer was identified; there is expertise in BER around somatic mutations.

Anderson explained that next steps on the charge could involve a workshop or roundtable format. **Hungate** will be reaching out to BERAC members to begin the process. Several BERAC members volunteered to assist with this charge.

Public Comment

None.

Hungate dismissed the meeting for the day at 5:23 p.m.

Friday, April 21, 2023

West convened the meeting at 8:30 a.m. The SC Statement of Commitment was shared, outlining DOE's expectation for professional behavior and commitment to a safe, diverse, and inclusive environment.

BERAC Subcommittee on Data Unification Framework: Update – Dr. Kerstin Kleese van Dam, BNL

[Presentation posted]

Discussion

The importance of the ontology of standardized metadata was emphasized. **Kleese van Dam** stressed the importance of this as well, otherwise the data will not be used.

West commented the RFI on a more Unified Data effort within BER is available on the BER webpage.

A BERAC member mentioned light sources as a source of data; are they included? **Kleese van Dam** confirmed they are.

An individual asked about interaction in this area with the rest of world and whether international linkages will be made. **Kleese van Dam** confirmed the subcommittee will be looking at how to best facilitate discussions and create tie-ins with international data sources.

Will there be efforts to test the usability of this information with groups in specific geographical regions where data is currently lacking? **Kleese van Dam** appreciated this idea and pondered reaching out to other agencies and private companies using an interface to deliver data to a new audience.

Have intelligent, automated tools and techniques been considered to scale the system and make it easier for the adoption for emergent data? **Kleese van Dam** stated large data producers automate metadata attribution but for smaller scales, a new solution is needed; it is not viable to

rely on scientists typing in the metadata. There is not a good solution right now, but there is hope AI/ML can help with this in the future.

A BERAC member told attendees that the BER data activation barrier is too high for trainees. New tools must be user friendly. **Kleese van Dam** concurred with this sentiment and will be looking for groups willing to discuss this issue.

DOE SC Integrated Research Infrastructure – Dr. Ben Brown, ASCR Facilities Division Director

[Presentation posted]

Discussion

An individual shared the challenges of integrating data from earth systems models, process models, and field campaign observations and was encouraged by the work being done at ASCR. **Brown** appreciated these comments and emphasized there is no presumption of ASCR owning the data. Data ownership and stewardship is paramount. Working with BER has shown the difficulties of providing computing power and resources for temporary use cases that have well-defined start and end dates.

A commenter agreed the three presented motifs are spot on, but the motifs also need to be integrated and not standalone. How will ASCR and BER be able to collaborate around this in the next five years? **Brown** emphasized data ownership and visible roadmaps. ASCR and BER have not been strategically connected and need to deal with the contention of resources in real-time cadences. ASCR cannot own every mission, and the domain sponsor sometimes must own the stewardship.

A BERAC member asked who the main user is for ASCR data and whether there is a good mechanism for increasing data usability. **Brown** explained ASCR facilities are open user facilities for the nation. The National Energy Research Scientific Computing Center (NERSC) serves approximately 8,000 users and 1,000 projects annually. The Argonne Leadership Computing Facility and Oak Ridge Leadership Computing Facility are nationally mandated resources with broader user bases, including the private sector. The users are so broad that it defies generalization, ranging from interagency partnership to large manufacturing firms.

BER Data Activities: KBase, NMDC, ESS-DIVE, ESGF – Dr. Adam Arkin (LBNL), Dr. Emiley Eloe-Fadrosh (LBNL), Mr. Shreyas Cholia (LBNL), Dr. Forrest Hoffman (ORNL) [Presentations posted]

Discussion

Questions were held for the final discussion period of the day.

Hungate dismissed the meeting for a break at 10:48 a.m. and reconvened at 11:00 a.m.

BER User Facility Data Activities: ARM, JGI, EMSL – Mr. Giri Prakash (ORNL), Dr. Kjiersten Fagnan (JGI), Dr. Ratna Saripalli (PNNL) [Presentations posted]

Discussion

An attendee commented there are a lot of activities in terms of data but only through small efforts; there must be standardization for data across all BER enterprises. **Hungate** agreed. BERAC members and attendees were challenged to picture what the best-case scenario for data efforts would look like in five years and then to start working towards that.

An individual commented many journals are asking PIs to upload all their data and was intrigued by Arkin's mention of the partnership with the American Society for Microbiology, which runs many journals.

A BERAC member was curious about integrated data sets and the possibility of attribution happening on the data center and operations side. **Prakash** gave the example of the MO-SAiC expedition, where the data partners and scientists worked together to create the attributions. **Cholia** mentioned the work being done through the Complex Citations Working Group at the Research Data Alliance (RDA).

An inquirer asked about ARM developing large-scale data in single column mode to facilitate evaluation of the models and create a dialog between the model and the modelers. **Prakash** agreed for the need to reduce barriers for modelers; ARM has been working methodologically on how to improve data preparedness.

The interoperability between data repositories was questioned; is DOE looking at what is and is not working in this area? **Kleese van Dam** said this is not being done at that scale but there are efforts to accelerate the integration of data. **Arkin** confirmed this is a priority of the Systems Biology Knowledgebase (KBase); discussion have started on a Data Transfer System (DTS) to move and validate data, which will hopefully be generalizable.

KBase was commended for the efforts on data attribution and credit. There is a fine line between giving credit and not hindering science.

A BERAC member discussed data credit and reuse; citing data must be incentivized moving forward. An observation was made about data curation by experts in the field. This might look like preparing integrated ARM data sets available for relevant questions. A follow-up comment was made about DEI assessments of the available data resources.

An attendee urged a more ambitious view on curating, archiving, and evaluation of research. The principles of pushing for more unified data effort is great start to addressing what might be the current existential crisis in the sciences. Another emphasized the balance of making these tools successful but not having them evolve so fast that the user base is lost. Similarly, there must be incentives to properly credit data sources.

An individual suggested a briefing on the low-dose radiation charge. **Hungate** acknowledged this idea and confirmed BERAC is thinking about how to address this charge.

It was suggested BERAC think more about systems and cascades across scales. **Hungate** liked this idea.

Public Comment

None.

Hungate adjourned the meeting at 12:11 p.m.

Respectfully submitted May 2, 2023 Drew Nitschke Science Writer, ORISE