

### Palladian Room, Omni Shoreham Hotel 2500 Calvert Street NW Washington, DC 20008 Thursday, February 16, 2012 at 9:00 am.

### Agenda Thursday, February 16, 2011 (Day One)

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9:00	Office of Science Update	3	William Brinkman, Director, Office of Science
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10:30	State of BER Report	16	Sharlene Weatherwax, BER Associate Director
11:30	Break	20	
11:45	Joint Genome Institute (JGI) Update	21	Eddy Rubin
12:15	Environmental Molecular Sciences Laboratory (EMSL)	23	Allison Campbell
12:45	Lunch	26	
2:15	Knowledgebase Discussion	26	Adam Arkin
2:45	Basic Energy Sciences	30	Harriet Kung
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4:00	Continued Discussion of Charge: Technology Implementation for Long Term Vision	34	
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#### Agenda Thursday, February 17, 2011 (Day Two)

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8:30	Climate and Environmental Sciences Division Update Biological Systems	39	Gary Geernaert Susan Gregurick
9:30	Science Talk "What Can We Learn From Climate Models?"	43	Judith Curry, BERAC Member
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#### Dr. Gary Stacey, Chairman, was presiding.

### **ANNOUNCEMENT**

Dr. Stacey thanked everyone for being prompt and advised that Dr. William Brinkman would be giving his Office of Science update including details on the 2013 budget request first as he had obligations elsewhere and would unfortunately have to leave after his presentation.

### **ROLL CALL**

#### **Committee Members Present:**

Dr. Gary Stacey, Chair Dr. Dennis Baldocchi Dr. Janet Braam Dr. Judith Curry Dr. James Ehleringer Dr. Susan Hubbard Dr. Andrzej Joachimiak Dr. L. Ruby Leung Dr. Gerald Mace Dr. Joyce E. Penner

#### **Committee Members Absent:**

Dr. Gregory Petsko Dr. Gaius Shaver Dr. Ray Wildung Dr. David A. Randall Dr. Warren M. Washington

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Dr. Karin Remington Dr. G. Philip Robertson Dr. Gary Sayler Dr. Martha Schlicher Dr. Jacqueline Shanks Dr. Herman Shugart Dr. James M. Tiedje Dr. Judy Wall Dr. Minghua Zhang Dr. Huimin Zhao

### **Designated Federal Official (DFO):**

Dr. David G. Thomassen

### **OFFICE OF SCIENCE UPDATE**

#### Dr. William Brinkman, Director, Office of Science

- Explained that he had been in charge of the Department of Energy (DOE) CFC (Combined Federal Campaign) and had to leave early to present awards to volunteers at the final awards ceremony. He apologized for having to leave early.
- Noted that the budget generally had its high and low points but he considered that it was reasonable for BER (Biological and Environmental Research).
- Emphasized that the Office of Science (SC) is a major player in scientific research in the U.S. Stated that:
  - Over 100 Nobel Prizes have been received including by SC scientists, including one in 2012.
  - SC provides 45% of basic research in the physical and energy-related sciences.
  - SC supports 25,000 PhD scientists and graduate students and 300 staff at 300 institutions.
  - SC provides the world's largest collection of user facilities to 26,500 users.
- Stated that President Obama had been an outspoken advocate on behalf of science and technology and provided a significant quote from the State of the Union Address. Noted that the president emphasized that innovation demanded basic research and that "Nowhere is the promise of innovation greater than in American-made energy".
- Reminded that science is the basis of technology and underpins America's energy future.

- Stated that continuing progress in science and technology depended on continuing advances that itself needed replenishment from basic research.
- Noted that highly trained scientists and engineers trained in modern science and technologies and with access to the best tools are required to invent the future.
- Added that the SC had an arsenal of science capabilities including major scientific user facilities, national laboratories and researchers breaking down barriers to new energy technologies.
- Explained that to meet the national energy needs they had focused capabilities through the Bioenergy Research Centers (BRC), the Energy Frontier Research Centers, the Combustion Research Facility, the Joint Genome Institute (JGI), the five nanoscience centers and the two new Energy Innovation Hubs, one researching fuel from sunlight and the other, batteries, that came out February 1st.
- Stated that there were three themes in science for clean energy: nanotechnology, biotechnology and modeling and simulation.
- Described:
  - Materials and chemical processes by design: using nanoscale and mesoscale structures for scientific advances and manufacturing innovations in solar energy conversion; clean energy electricity generation; battery and vehicle transportation; and carbon capture use and sequestration. Noted that numerical simulation was a critical part of materials research.
  - Biosystems by design: targeting the development of synthetic biology tools and technologies and integrative analysis of experimental genomic science datasets for the design and construction of improved biofuels and bioproducts. Noted the importance of DNA sequencing but also protein structure and function. Stated that the DOE sees this area as important because of microbes and plants for biofuels and how microbes and plants impact climate.
  - Modeling and simulation: using SC's Leadership Computing Facilities and production computing facilities to advance materials and chemistry by design and broadly address energy technology challenges.
- Discussed examples of materials and chemistry by design and noted the use of computers to survey large numbers of different compounds and reviewed the large number of materials that they had simulated.
- Discussed examples of biosystems by design including predictive design of innovative natural and hybrid systems for clean energy production and the synthetic design of plant and microbial systems advancing scientific understanding for the sustainable production of biofuels and bioproducts.
- Reviewed the SC FY 2013 Budget request to Congress and noted:

- Budget was increased for Biological and Environmental Research, for Basic Energy Sciences and Advanced Scientific Computing Research.
- Due to those increases funding had been reduced for the remaining three; Fusion Energy Sciences, High Energy Physics and Nuclear Physics.
- Stated that the main functions of the SC were running the national laboratories and overseeing the science. Discussed the different programs.
- Reviewed Advanced Scientific Computing Research
  - One aspect of Advanced Scientific Computing involved keeping the SC at the forefront with the latest or next-generation computing machines. He said they have the IBM Blue GeneQ, a 10petaflop machine that would come to Argonne National Laboratory (ANL) this year. He said the Cray machine at Oak Ridge National Laboratory (ORNL) would be upgraded to between 10 to 20petaflops.
  - Noted the high cost of the new computing machines and added that they manage costs by using lease-to-buy.
  - They were considering how to deal with exascale and reviewed the differences with petaflops. Noted that the speed of computers which was no longer increasing. He discussed the other problem which was if one extrapolated the current technology you would get two things, the power you would need is a gigawatt and the other was that microprocessors would make statistical, not defect errors. These factors make it a more complicated arena in which to compute. He noted that with respect to power they were working with the industry. With regard to the errors they were working with mathematicians and computer scientists considering the problem.
  - The second aspect concerned co-design teams and this meant a bringing together of people interested in solving a certain problem, for example, fluid dynamics. They then couple these people with scientists and mathematicians who understand how to use parallel processing machines so that real simulations can be done.
  - They had three teams and will put two more together in 2012.
  - They wanted to keep continuing to fund the SciDAC (Scientific Discovery through Advanced Computing) and INCITE (Innovative & Novel Computational Impact on Theory & Experiment) programs to ensure that they were making good use of these computers.
  - One of the issues that they were trying to negotiate was how to interface to industry with these high-powered computers. He noted that the SC can frequently solve a problem that a company is unable to do, impacting strongly on the company.

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- There was a meeting in March in which they were bringing together the computer scientists from the national laboratories with the industry people to develop an exchange.
- Some examples of companies where the SC has worked with companies was given such as the design of blades in turbines for GE and the design of using plastic boxes on the bottom of longhaul trucks to reduce air drag and save on fuel costs.

### • Reviewed Basic Energy Sciences:

- A substantial amount of funding was put into this area because of the connection to batteries, solar cells and windmills.
- Materials play a dominant role in a lot of the technology.
- Trying to enhance their efforts in clean energy and work closely with the Office of EERE (Energy Efficiency and Renewable Energy) with global energy work.
- Working on materials by design and several years ago started the construction of NSLS II (National Synchrotron Light Source II) that is a new synchrotron at the Brookhaven National Laboratory (BNL) and they are in the process of completing that.
- The synchrotrons are heavily used and the biology community comprises 50% of the users.
- The APS (Advanced Photon Source) is being upgraded.
- LCLS (Linac Coherent Light Source) is being expanded, a new thrust in the use of electron beams. This has created the first X-ray laser. Previously the X-ray laser was amplified but that is not what is required so they have managed now to create an X-ray beam that is then stimulated, it simulates more emission that gives a narrower line closer to a pure X-ray line.
- There are 46 Energy Frontier Research Centers (EFRCs) in 35 states with a large number of investigators and students. Some of the examples of the work were given including growing silicon rods.
- The Fuels from Sunlight Hub was just being started. The object is to create synthetic photosynthesis. Although not a new concept it is believed progress in catalysts and physical chemistry could enable new things to be done.
- For LCLS-II a second beam line so they have more X-rays and to broaden the region of energy in which an X-ray laser can be created.
- The upgrade at the APS (Advanced Photon Source) will give high-energy X-rays with high resolution.

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- Stressed the political and economic importance of the assistance that the field of basic energy sciences affords industries.
- Reviewed Biological and Environmental Research:
  - Noted the importance of plants and microbial systems and the development of new molecular toolkits for systems and synthetic biology research.
  - Support continues for Bioenergy Research Centers that received strong reviews.
  - The Joint Genome Institute is a tremendous success. Noted that they were trying to create a second campus and laboratory at Berkeley where the biology part of the laboratory would be based. The benefit of having the JGI and laboratories situated in one central location was discussed.
  - Noted the work accomplished in the area of climate.
  - Thought that ARM (Atmospheric Radiation Measurement) had played an important and central role in understanding clouds and aerosols.
  - The three bioenergy research centers, BESC (Bioenergy Science Center) at ORNL are looking at lignin biosynthesis genes in switchgrass, JBEI (Joint Bioenergy Institute) using a synthetic biology toolkit to construct microbes to produce biofuels from switchgrass and the GLBRC (Great Lakes Bioenergy Research Center) are researching at crop and soil management in relation to greenhouse gas emissions.
  - Noted the JGI and its advances in metagenomics, important because of challenges in the culture of microbes in isolation from natural communities to study sequencing.
  - The improvement of climate modeling including models studying the Arctic sea ice and the improvements to the Community Earth System Model. Described the work at Lawrence Livermore National Laboratory (LLNL) where inter-model comparisons are done and used by the IPCC (Intergovernmental Panel on Climate Change).
  - Summarized the establishment of key partnerships with other federal agencies to ensure that climate research has an improved coupling to the energy world. Partnerships mentioned included the Coordination of Climate Research through the United States Global Change Research Program (USGCRP) and the Joint USDA-DOE Plant Feedstock Genomics for Bioenergy.

#### • Reviewed Fusion Energy Sciences:

• A main issue for Fusion Energy Sciences is ITER (International Thermonuclear Experimental Reactor) that is entering its construction phase without sufficient funding. The European Union

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pledged €1billion a year for the next two years and the United States pledged \$150 million so that issue has to be considered within the next few months.

 The domestic program was discussed with the National Spherical Torus Experiment (NSTX) upgrades at Princeton.

#### • Reviewed Nuclear Physics:

- The main issue is they have not been able to obtain large increases in funding to continue with ongoing construction plans for facilities including one for isotope beams in addition to maintaining Brookhaven National Laboratory.
- SC will wait for the community to come back to them to advise the course of action.
- The nuclear physics group has taken on the responsibility of maintaining isotope availability. They have brought together and have coordinated the users and suppliers of isotopes and radioisotopes.

#### • Reviewed High Energy Physics:

- During the next 12 months they will start up running the LHC (Large Hadron Collider) and hopefully be able to come to some conclusions by the end of 2012.
- The LHC is running well and the total luminosity it has generated is equal to the total luminosity that the Tevatron generated during its life.
- Neutrino experiments are a major issue and much is still not known.
- Cosmology is also of interest concerning knowledge of dark matter and dark energy that makes up 95% of the universe.
- The area of accelerator technologies is also an area of research for high energy physics and they have been the source of a lot of the advances in accelerators.

### WELCOME AND INTRODUCTIONS, BERAC

Dr. Stacey explained that introductions were made to enable the members of BERAC to get to know each other. He asked that they introduce themselves and feel free to also mention any current research that they felt was of interest or general matters with which they had a concern.

Dr. Gary Sayler introduced himself and said he was from the University of Tennessee (UT), a
professor of microbiology and director for the Center for Environmental Biotechnology. Added that
he also directs a joint UT Oak Ridge Institute for Biological Sciences. Noted that his areas of research
were broad, molecular and environmentally-related work. Discussed BERAC and noted that at times
committee members could make more of a contribution if more was known about the 'ins and

outs', working conditions of the programs and more transparency. Noted that this year in particular it had registered as major programs in BER were facing funding challenges and it had caught many members, himself included, off guard. Asked if there was a way that more information could be provided so that the advisory relationship between BER and BERAC could be improved.

- Dr. Joyce Penner introduced herself and said she was from the University of Michigan and works on climate models and aerosols, representations from climate models and interactions with clouds. Added on a research note that she had discovered an interesting way to use satellite measurements to calibrate cloud/aerosol interactions.
- Dr. Andrzej Joachimiak introduced himself and said he was from Argonne National Laboratory and also a professor from the University of Chicago. Added that he also heads the Center for Structured Biology and the Midwest Center for Structural Genomics. Discussed his research and noted that they had completed the design of a new facility. Added that he was closely involved in the upgrade of the APS and noted that they want to expand biologic capabilities to study protein characterization. Stated also that it included systems biology and membrane studies, exciting projects done in collaboration with DOE projects. Stated it was funded by BER and presented further details on their discoveries of compounds.
- Dr. Susan Hubbard introduced herself and said she was at Lawrence Berkeley National Laboratory and added she was the deputy division director of the Earth Sciences Division. Noted that her focus was on subsurface biogeochemical processes, hydrological processes and their couplings using geophysical data. Noted that the most interesting project she had been involved in during the last year was the scaling issue within her own research group focusing on the subsurface and as part of the Next Generation Ecosystem Experiment (NGEE) team focusing on carbon and ecosystem science. Added that this involved both developing and testing methods to take the understanding they would develop at the small field scale up to a large scale. Described not just the common questions and approaches but also added the fact that her group had developed an approach that leverages on geological units. Explained the process in further detail and commented that testing was done successfully at the contaminated Savannah River site. Noted that it needed to be tested at various sites but might offer a new paradigm. Noted that in the NGEE team they had come up with another unit for the scaling and subsurface geologic units but also hydrogeomorphic units distributed in the landscape. Described further the scaling framework in detail and noted she had been thrilled to be part of a team involved in these initiatives.
- Dr. Philip Robertson introduced himself and said he was from Michigan State University and was an ecosystem ecologist, carbon and nitrogen biogeochemist. Added that recently he had been working on scaling issues and in particular scaling the greenhouse gas footprints of bioenergy systems up to the regional and national scale and in particular asking questions about whether there are sufficient marginal lands in the U.S. to support the biomass production, necessary to make meaningful

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contribution to feedstocks and assessing the greenhouse gas implications of that, especially with respect to carbon footprint and nitrous oxide footprints in particular.

- Dr. Judy Wall introduced herself and said that she was from the University of Missouri in Columbia, MO in the Biochemistry Department. Added that her research focuses on environmental microbes that are anaerobes, sulphate-reducing bacteria in particular. Stated that one issue on her radar screen has been the education of the next generation and she wondered if they were being prepared sufficiently and would they be able to step into the research that her generation would leave behind.
- Dr. Jacqueline Shanks introduced herself and said she was a professor in chemical and biological engineering at lowa State University. Added that her focus was measuring reaction rates in living systems, microbes or plants. Stated that she was a research leader in microbial metabolic engineering for an engineering research center that has a goal to produce bio-renewable chemicals and fuels. Described several courses she teaches involving the fate and lifetime of chemicals in the environment. Added that she was interested in the discussions relating to scales on the soil, water and air and incorporating biology into that. Stated that her training was broad as she was also an engineer.
- Dr. James Ehleringer introduced himself and said that he was from the Department of Biology at the University of Utah. Added that he was an ecologist in ecosystem science so noted that he was interested in carbon cycles and water cycles particularly fluxes in and out of ecosystems in the Western U.S. Noted that he had a growing interest in applying what is learned to natural systems, to understand urban systems and urban sustainability and development. Said that he felt there was a need to jump from physics and biology into social systems and the human-dominated systems that he saw as an important role. From an academic standpoint he said that they had developed an enviro-van, a vehicle that allowed them to take their place-based sites, such as one might have in an ARM site and make it mobile so that models could be tested. Added the vehicle allowed them to obtain precision trace gas analysis and stable isotope analysis and radio-carbon analysis in real time, producing graphics.
- Dr. Dennis Baldocchi introduced himself and said that he was a professor of biometeorology at UC, Berkeley. Added that his interests were measuring trace gas exchange between ecosystems and the atmosphere. Noted that he had been involved with the Ameriflux Project, a DOE project, since its inception with a network of approximately 50 sites making long-term measurements of trace gas exchange for forests and croplands. Added that his most recent work was becoming involved in methane exchange as they were trying to do some work on restoration in the California delta. Explained that the concept was if the drained peat lands were re-flooded they could be big carbon sinks; however, once flooded microbes would take over and huge amounts of methane could be produced. Noted that there was a whole new generation of sensors that was allowing them to make continuous measurements at field scales. Noted that they were also working on semi-air ecosystems

and they were seeing again the interesting role of microbes in the field scales. Explained the process and said that the sun breaks down the organic matter, makes complex carbohydrates into sugars for the microbes, the first rains comes and they see huge pulses of  $CO_2$  coming out of the ecosystem. Stated that he was new on BERAC and looked forward to working with everyone.

- Dr. Gary Stacey introduced himself and said he was from the University of Missouri and a professor of plant science and was affiliated with the Department of Biochemistry. Added that his PhD was in microbiology but had evolved over time and he considered himself a plant scientist. Stated that one of their current interests in the lab was plant microbe interactions both beneficial and pathogenic, a broad program. Noted he also is involved in the area of public policy so he founded a not-for-profit in Missouri focused on energy policy areas. Added that on a national level he is also involved in public policy related to plant science. Explained the importance of committee members appreciating the opportunity of interacting with the SC and offering their opinions on important areas during discussions initiated by charges given by the SC. Suggested that members could be more proactive in those areas and asked them to consider cutting-edge areas that would impact beneficially the BER mission going forward.
- Dr. Minghua Zhang introduced himself and said he was from the Stony Brook University of the State University of New York and added he was a professor in atmospheric science. Added that his research is in climate modeling particularly cloud convection, boundary-layer turbulence. Stated that at the present time he was leading an international project studying cloud feedbacks in climate models and he also co-chairs the Atmospheric Modeling Working Group of the Community Earth System Model. Noted he was also interested in doing research regarding integrating heterogeneous data from different platforms into a physically consistent format for modeling of systems.
- Dr. Herman Shugart introduced himself and said he was the W.W. Corcoran Professor of Natural history at the University of Virginia. Added that his long-standing interest has been in understanding the dynamics of the forest, forests worldwide and particularly focusing on climate change affecting feedbacks between the forest and atmospheric processes of various sorts. Added he was originally a zoologist. Noted that lately his group had been working on strong feedbacks between terrestrial surface and more or less decadal-type timescale climate change notably in Russia.
- Dr. Janet Braam introduced herself and said she was the Chair from the Department of Biochemistry and Cell Biology at Rice University in Houston, Texas. Noted she had been involved in one project with a graduate student that had resulted in the publication of a paper in PNAS (Proceedings of the National Academy of Sciences). Added that her general area of interest concerned how plants respond to stress. The project concerned research into the significance of a large number of genes that would be regulated by the circadian clock in plants. About one third of the genome is regulated by the clock. The experiments looked at the physiological significance of plants in two ways, plants that were synchronized with the insects were highly resistant to herbivores and those not synchronized with the insects were demolished and did not use the clock to defend against the

insects. She considered the relevance to BER research because they had also found the same was true for fungal infections. Added that for BER research the interaction between microbes and plants there might be other phenomena like the time of day that may impact these interactions. Added that this was something they should keep in mind when studying plant-microbe interaction.

- Dr. Huimin Zhao introduced himself and said he was a professor from the Department of Chemical and Biomolecular Engineering at the University of Illinois at Urbana-Champaign. Added he also had a joint appointment in chemistry, biochemistry, biophysics and bioengineering so his program was very interdisciplinary where the focus is on enzyme engineering, metabolic engineering and broadly, synthetic biology. Explained that one of the main research themes in his lab is the engineering of bugs to utilize biomass to produce biofuels, chemicals and drugs. Dr. Zhao gave some detailed examples of his laboratory research.
- Dr. Ruby Leung introduced herself and said she was a scientist at the Pacific Northwest National Laboratory, a climate modeler and interested in looking at different processes and how they are represented in climate models. Added the models are also used to test different hypotheses about what is going on with the climate system. Noted that there were two pieces of work that she was excited about, one was that they had been using some uncertainty quantification methodology to look at how land surface models are sensitive to different parameters and she explained some of their results. Added that another piece of their work was to look at aerosol effects on cloud and precipitation using data from ARM over the southern Great Plains and over China and some results were explained.
- Dr. James Tiedje introduced himself and said he was a microbiologist at Michigan State University. Added that in recent years he had focused on microbial genomics. Noted that the microbe is important in the environment and more recently on metagenomics, the understanding of microbial communities from the gene level. Stated that he was currently involved in four metagenomic projects and three dealt with the soil environment and noted that they were dependent upon the JGI, an institute he considered essential for research in the new field of metagenomics of the environment. Dr. Tiedje noted that he would consider the most interesting thing for him is working with a talented group of scientists who have made major progress of assembling the complexity of the soil communities so they could interpret the function of the communities in more effective ways.
- Dr. Judith Curry introduced herself and said she was the Chair of the School of Earth & Atmospheric Sciences at the Georgia Institute of Technology. Added that she would not go into detail about her research as she was presenting the following day. She did mention that historically her research had been in the area of cloud and sea ice processes and how to improve the treatment of these natural elements in climate models. Added that over the past five years her research had undergone a substantial transition and was currently working in two broad areas, one is the applications of weather and climate information and modeling information and she had formed a company called

Climate Forecast Applications Network with the major target being the energy sector. Added that they had recently received a new DOE-STTR (Department of Energy – Small Business Technology Transfer) grant they were recently awarded to look at wind energy, and extended range predictions. She added her second area of interest involves a broad range of issues concerning the science policy interface.

- Dr. Gerald Mace introduced himself and said he was a professor of atmospheric science at the University of Utah and noted that he was interested in the processes that move water through the climate system. Added that his research involves a lot of time looking at remote sensing data and added that recently he had been using aircraft data collected by the ARM program to validate NASA (National Aeronautics and Space Administration) satellite retrievals and he had been using aircraft data collected by NASA to validate ARM retrievals, so he was very busy working across agencies.
- Dr. Martha Schlicher introduced herself and said she was with the Monsanto Company. Added that Monsanto was a global agricultural company and the largest seed company in the world. Stated that she led the overall bioenergy and bioindustrial efforts and another area in that she worked was on improving the data and quality of models that are used to inform policy and to guide research needs in the whole area. She gave an example including working collaboratively to fund a model at Washington University in St. Louis to understand what would be required technically, economically and considering both technology and biology to develop commercially-viable algae as a feedstock for biofuels.
- Dr. Karen Remington introduced herself and said she was from the National Institutes of Health (NIH), the Institute of General Medical Sciences in particular. Noted that her training was in mathematics and computer science and her connection to BER work is previous genomic science research completed before coming to NIH. Added that since the last meeting the Center for Bioinformatics and Computational Biology had inherited a large chunk of the programs from the recently-dissolved National Center for Research Resources (NCRR). Stated that they had received approximately \$50 million worth of research centers in biomedical technology from NCRR. Stated that the process of integration was ongoing. Added that for the last nine months she had been cochair of an interagency working group on big data, trying to craft a big data initiative.

### **COMMITTEE DISCUSSION – GRADUATE SCIENCE FELLOWSHIP PROGRAM**

Dr. Stacey noted that as Chair he was using his prerogative to open discussion about the SC Graduate Science Fellowship Program. He said that in the FY 2013 budget, the program had received no funding. Dr. Stacey added that he had discussed this with the Chairs of the other SC advisory committees and that general concern had been expressed. It was mentioned that the Office of Management and Budget (OMB) considered the program more aligned to the National Science Foundation (NSF) rather than the DOE. Following the decision to not fund the program Dr. Stacey noted that he wanted to open this for discussion. Members were asked to consider if the drafting of a letter of support for the program might

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be appropriate and might have some impact in either restoring the program for FY 2013 or a subsequent financial year.

Dr. Stacey was asked the scale of the program and how many students were involved. Dr. Julie Carruthers (SC) stated that in the first year of the program, FY2010 150 graduate fellows were funded, 80 funded with the Recovery Act and 70 funded with base funds. She added that they had a current solicitation right now and noted that they would fully fund approximately 50 fellows.

A member asked about the supposed connection of the NSF to the DOE for the program. Dr. Stacey responded it was more hearsay than fact but added that there appeared to be more support for programs of that type in NSF as opposed to DOE.

A member stated that graduate students are funded two ways, through grants and contracts, and through fellowships and noted that she preferred the fellowships as it was more tied to the students giving them room for innovation as opposed to doing research for a specifically-funded project. She added that she preferred the merit-based model of the fellowships.

Another member stated as the program had begun with funding from the Recovery Act, he wondered whether it was viable as an independent program. He noted that they had something analogous in NSF called REUs (Research Experiences for Undergraduates) where if you have existing funding you can apply for additional funding for undergraduates. He added if the issue was that the program was small and could not stand on its own then he suggested that researchers who have research grants can apply to a common pool for graduate funding.

Another member mentioned that the program had in the past funded international students and he said that the NSF would not fund foreign nationals. He thought this would make the pool smaller and he added that as tuition costs were rising fewer and fewer foreign students were being recruited.

Dr. Carruthers confirmed that the program was for U.S. citizens only.

A member noted that the graduate fellowship program was independent of the science that is funded by the program offices. He clarified that a solicitation would go out for the broad areas of science funded but there would be no requirement that the students work for researchers funded by the DOE, just that the research be related to a DOE SC relevant project. He explained it was more complicated than saying one could cut back on the grants and give it to the students as many of them are not working with researchers funded by SC-funded scientists.

A member asked if there was any available data to assess the success of the program. Dr. Carruthers responded that last year was the first year it was re-started so the first year's students were just finishing their first year of funding. Another member stated that there was anecdotal information about students who had published and presentations they had given but confirmed again they were in their second year.

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A member asked if there was a rationale given for cutting the program. She asked if it was purely a budget limitation or some kind of disconnect between what was funded and the projects. A member responded that it was basically a decision made by the OMB and it may have been thought that it was not a mission for the DOE but that it might belong in the NSF.

A member stated that she did not feel that the NSF would not like to be responsible for funding DOErelated graduate fellowship programs. She thought that they would not do that and if DOE did not fund it, it would not be done.

A member stated that there were ways through inter-agency agreements to fund a pool of students or projects where BER could provide funds. He thought that they should look into how budget constraints are starting to affect training students and post-docs.

A member stated that at his university fellowships are immune to overhead and for students immune to taxes so he thought they were a cost-effective way to pay for a student. He also noted having meritbased strong students involved with the DOE program would plant seeds for future opportunities. He thought that professors might have a very bright student looking for funding who was not involved with the DOE. He thought that using fellowships would save a considerable amount of money and would also create a good level of diversity. He endorsed the idea of writing a letter to present their case.

A member noted that for recruiting the best for the national labs meant getting students from graduate school and post-docs and she said there was no program that would help them with the exception of researchers' own contracts.

A member agreed that it would be a loss to lose the fellowship program but noted that Dr. Brinkman might ask that they identify where funds could come out of existing programs if they wanted to save the fellowship program.

A member suggested they write a letter recommending a reconfiguration of the program stating that it should be used to support collaboration between universities and the DOE labs, in other words, some concrete steps with the recommendation. Dr. Stacey stated that micro-managing the program might not really be their role but they could express a general support for the program.

Dr. Stacey said they did not necessarily require a vote but asked if anyone opposed the idea of sending a letter to Dr. Brinkman giving the advisory committee's support for the program and asking that everything be done to try to maintain it. He noted that no one opposed it and asked for volunteers to draft the letter. Dr. Remington and another member volunteered. A sub-committee was created of the two plus Dr. Stacey and he noted that it would be circulated to all members before it would go forward. Dr. Stacey confirmed he would advise the Chairs of the other advisory committees of their decision.

Dr. Stacey stated that there would be sufficient time for committee discussion and he wanted members to consider issues that they wanted to bring forward. He said that he wanted BERAC to become a more proactive committee. A member asked if a decision had been made about the number of meetings

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being held each year. Dr. Stacey responded that had been decided and their packages showed the next meeting was in June, so three meetings per year.

Dr. Remington asked if Dr. Stacey could say anything further about his ongoing interactions with the other committee Chairs. Dr. Stacey responded that when he came on as Chair he was told that in the past there had been an executive committee made up of all the Chairs. He noted that it had become inactive and when he was first named Chair he thought he might benefit from initiating a regular communication with the other Chairs and he had done this. He stated that they had had about four telephone calls and the group had recently discussed the 2013 budget and how it would impact certain areas. He added that the group wanted to be useful to the SC and identify cross-cutting themes.

### **STATE OF BER REPORT**

#### Sharlene Weatherwax, Associate Director, Office of Biological and Environmental Research

- Welcomed everyone to the meeting and noted the many new faces and as a consequence was structuring the meeting differently by presenting some basic background, overview and information.
- Outlined the structure within the DOE and noted some of the relationships that BER had with the SC and some of the applied offices and the NNSA (National Nuclear Security Administration).
- Outlined the structure of the DOE Office of Science and noted there were three areas:
  - Dr. Patricia Dehmar is the Deputy Director for Science Programs and helps to facilitate the interface between all of the program offices.
  - Another main area is Field Operations with the grant office in Chicago that manages financial assistance and contracts.
  - The remaining area is the Resources Management office involved in budget requests.
- Reviewed the structure and discussed the staff of BER.
  - There are two divisions in BER, the Biological Systems Science Division and Climate and Environmental Sciences.
  - Within each of the divisions there are program elements and many are collaborative.
  - Program Managers are encouraged to engage with their colleagues and the science community so that there is a vibrant level of communication and they can cross-fertilize. The increase in the number of meetings in BER was to further encourage discourse.
  - Detailed the program elements within the two divisions. Biological Systems Science: Genomic Science; Radiological Sciences; Joint Genome Institute; and Structural Biology Infrastructure and

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Climate and Environmental Sciences: Atmospheric System Research; Environmental System Science; Climate & Earth System Modeling; Atmospheric Radiation Measurement Climate Research Facility; ARM Climate Research Facility and Environmental Molecular Sciences Laboratory (EMSL).

- Reviewed highlights of several of the program elements of each division beginning with Biological Systems Science:
  - Genomic Science highlights included understanding the nature of biomass, the design and metabolic engineering of microbial systems for developing biofuels synthesis and developing the Knowledgebase, a data collection framework.
  - Radiological Sciences highlights included research in radiochemistry and radiotracer development to develop new methods for high resolution imaging, working relationships with NIH and Nuclear Physics.
- Reviewed some program elements of Climate & Environmental Sciences.
  - Climate & Earth System Modeling major element being worked on here is modeling at various scales. Goal is to develop models with strong theoretical foundations and to be able to use them to improve representations of key climate processes. Want to develop diagnostic methods and tools to evaluate the models.
  - Atmospheric Systems Research Tied to the output from the ARM facility and to assist in the understanding of atmospheric processes.
  - Environmental Systems Science Provides scientific understanding of the effects of climate change on terrestrial ecosystems including global carbon cycling and the role the subsurface plays. Includes support for the Arctic Next Generation Ecosystem Experiment (NGEE). A second NGEE has been initiated in the tropics.
- Reviewed the BER Scientific User Facilities that include the Joint Genome Institute, ARM Climate Research Facility and the Environmental Molecular Sciences Laboratory and stated that they represented BER's contribution to what the SC does to reach out to the scientific community including users at academic institutions, industry participants or international users. Stated that access is through application, peer review and at no charge. Tools are provided to researchers to bring ideas forward, test them and share results with the community through publications.
- Reviewed some of the interagency activities and partnerships at three levels, planning, exchange of information and coordination including funding opportunity announcements.
- Described some interagency activities:

- In Biological Systems Science Key partnership with the USDA (United States Department of Agriculture) for plant feedstock genomics research, Biomass Research and Development Board and radiobiology with NIH.
- In Climate and Environmental Sciences Key partnerships with the USGCRP, key interactions with the DOD (Department of Defense) like the Strategic Environmental Research and Development Program, joint climate modeling solicitation with the NSF and the USDA and the DOE.
- Discussed international partnerships with regard to ARM, GOAmazon and the Chinese Academy of Sciences.
- Discussed the FY 2012 BER appropriation and noted that a significant amount was allocated to research including research facilities.
- Will discuss what BER proposed for FY 2013. First reviewed the mission statement.
- Stated the BER scientific challenges as:
  - Understanding how genomic information is translated to functional capabilities, to understand, predict and design that.
  - Understand the role of the earth's biochemical systems from the subsurface to the atmosphere, terrestrial or ocean and to understand the roles to predict climate.
- Reviewed FY 2013 highlights:
  - Focusing on clean energy biodesign, plant and microbial systems.
  - Research and new capabilities to develop comprehensive environmental system models in the Arctic and the tropics, regions vulnerable to rapid climate change.
  - Continue support for Bioenergy Research Centers (BRC).
- Discussed the Bioenergy Research Centers:
  - Two onsite reviews and progress over four year period for each center.
  - Centers are complementary but each one is distinct.
  - The BRCs are reaching out to industry.
  - Asked BRCs to forge a strong linkage to the DOE Systems Biology Knowledgebase.
  - Encouraged to develop interactive websites.

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- Maintain their core research focus.
- Encouragement by BER to follow execution of the BRC research plans for years 5-10 following guidelines.
- Discussed a research highlight concerning two BRCs working collaboratively concerning the discovery of a new type of lignin and emphasized the equal importance of the goal of the development of biofuels with actual fundamental discoveries in science.
- A second highlight concerned the publication of research showing a correlation between greenhouse gases caused by humans to extreme participation events.
- Described some of the issues and goals concerning the NGEE-Tropics program.
- Noted that an award, the E.O. Lawrence Award was given to Tom Guilderson of the Lawrence Livermore National Laboratory.
- Reviewed BERAC and BER personnel changes.
- Thanked outgoing committee members for their dedicated service.
- Welcomed the new members to BERAC and added that she looked forward to much productive scientific exchange.

### **COMMITTEE DISCUSSION**

A member referred to the FY 2012 budget allocation and asked what proportion of the Biological Systems Science research went to the BRCs. Dr. Weatherwax responded that for BER overall funding is about half and half between the biology and the climate side. She referred to the graph and said for BSS Research it is \$218,000, then \$75,000 of that for the BRCs. A member asked about the idea of funding three large organizations for basic bioenergy research and asked if there any way to assess the efficiency or efficacy of that approach versus spending the same amount of money to fund small groups for individual research. She said the decision was made to go for large groups versus individual research. Dr. Weatherwax said that there was always a tension between science done on the scale of the BRCs and with a single PI (Principal Investigator) and BER's philosophy had always been that both are useful and they did not want to end one of them. Dr. Weatherwax added that there were still substantial contributions from individually funded PIs. She added that the NSF has had a long history of running some centers and they might have statistics to form an assessment.

Dr. Stacey noted the concern about the subsurface science program and where it is going and rumors about the field research centers. He asked if she could comment. Dr. Weatherwax responded that they had put forward their FY 2012 request and she said they were pleased with the appropriation but it came with some guidance and that meant mean BER had to make tough choices that are not obvious

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when the overall funding is reviewed. She said that they were held to maintain the same priorities in climate and bioenergy so they had to honor that request so if they were given funding they could only spend the money that way. That meant that tough choices had to be made in some programs and one of the programs in which they had to make a reduction was the subsurface biogeochemical research, sub-program area. She confirmed that they did not intend to get rid of that area of research but wanted to expand on what that research element is focused but more broadly. She confirmed that they have three field research centers and that in FY 2013 they intend to continue support of the research done using the integrated field research centers. Dr. Weatherwax noted however that they recognized their funding constraints in FY 2012 and FY 2013 and they probably could only guarantee being able to do that in a robust way at one site.

A member referred to the increase in the budget for environmental systems science and asked whether it was because of the ramp up of the NGEEs. Dr. Weatherwax responded yes, that they intended to continue support of NGEE Arctic effort and then also to initiate the planning for a new effort in the tropics. She said that they hoped to get that off the ground in FY 2013.

A member referred to the BRCs and noted that they were interdisciplinary, required a lot of management and asked if there was a mechanism for selection of new components at each of the centers that might or might not be working well. Dr. Weatherwax responded that that was part of what the reviews evaluated. She added that each center had a management plan with a formal process laid out on how they decide changes and priorities. She said that those were the mechanisms and some changes were also driven by new opportunities.

A member referred to the SBR program (Subsurface Biogeochemistry Research) and stated that she had heard that there would not be calls for proposals from investigators for two to three years. She asked if that was correct and if so, where would the scientists involved look for support for research. Dr. Weatherwax responded that they did issue a call at the beginning of 2012 and then when they realized that the budget mark did not look favorable they pulled that solicitation. She confirmed that there would not be a solicitation in 2012. She added that they were doing internal planning and they would not be able to say one way or the other about issuing solicitations. They would need to look at the progress of their science and the overall portfolio. She added that the SBR skills were transferable and that the member should talk to the program managers to see what would be in their portfolios.

### **BREAK**

The Biological and Environmental Research Advisory Committee recessed for a 15 minute break.

### JOINT GENOME INSTITUTE UPDATE

#### Dr. Edward Rubin, Director, Joint Genome Institute

- Stated he would be giving an update on current activities and where the Institute is going in the future.
- Noted that the JGI was first and foremost a user facility and they have approximately 1100 users • each year from 52 countries.
- Explained that the JGI differs from other DOE facilities as they have another set of users as all their research is available to the public as follows:
  - Maintain and curate every genome they generate and put the information on their databases. 0
  - Incorporate other data that is relevant, other genomes generated by other people.
  - Have tools to analyze the data that they generate.
  - Every month they have tens of thousands of visitors.
  - Have data and analysis tools at the JGI Informatics Systems.
  - Have a JGI Genome Portal and visitors in specific areas of microbial and metagenomes, plan and fungal.
  - An additional user is The Community Resource KBase.
- Stated that there had been approximately 200 papers published in the past year, 12 of which had been in Science and Nature. A few highlights of published papers are:
  - First complete genome from an uncultured single cell.
  - First report providing evidence of carbon fixation in the dark.
  - Data from the first assembly of switchgrass, a genome many of the Bioenergy Centers are focused on. The assembly is available. The paper has not been published as yet.
- Discussed the revolutionary advances in genomic technologies. Reviewed the scale of genomic sequencing and noted that several years ago they were discussing gigabases of sequence and now it is terabases of sequence and in the future, petabases of sequence, all within a five-ten year period.
- Noted that the JGI had been in existence for 13 years and now they are generating more data each year than their entire previous history.

- Stated that because of the revolutionary advances they were doing more science for less money so between 2009 and 2011 they had tripled the number of projects.
- Noted that they were generating massive data sets and need to draw on DOE high performance computing.
- Described a pie chart reflecting their FY 2012 budget distribution. Noted that now it cost less to generate sequence data and the costs now have moved to the analysis of the data.
- Stated that the JGI, for example in their Metagenome Program, has staff that assists users in helping them to design experiments and analyze their data.
- Added that they have changed the program to focus around specific focal areas rather than making it open to everyone interested in environmental issues. The focus areas are: Plant Microbe Interactions; Soil Carbon Cycling; and Aquatic Carbon Cycling.
- Discussed the Focus Area and JGI Coordination Workshop in which PIs and JGI staff meet and discuss issues.
- Discussed in detail one of the specified focus areas, plant microbe interactions. Stated that microbial communities: provide nutrients, protect from pathogens and stress, influence growth and sequester carbon. Described a variety of projects in that focus area one being the Casuarina, a salt-tolerant tree.
- Stated that another impact of the revolutionary advances was a heightened need for strategic planning at the JGI. Advised that currently they have a 2010-2014 strategic plan and they are in the process of developing a 10-year strategic vision.
- Described the current roadmap for 2010-2014:
  - Input came from two National Research Council (NRC) Reports that looked at plant biology and the science of genomics and they recommended large-scale projects to both deepen and broaden the genomic surveys of microbes and plants.
  - JGI is in the midst of the roadmap and in the process of first: systematically developing genomic resources for bioenergy relevant plants, algae and fungi, and secondly genomically characterizing the broad diversity of both cultured and uncultured microbes.
- Described the ten-year vision for the GJI and the draft would encompass: user community input; external expert scientific community input; and BER grand challenges.
- Noted that a draft plan had been created using that input and would be refined over the next eight months.

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- Reviewed the draft plan:
  - The historic core business has been: experimental data generation sequencing; data interpretation – assembly of sequence data; and user interactions – interactive data platforms.
  - The criteria, critical to the DOE's long-term vision, critical to the JGI user community and of a scale or complexity that needs to be located at a facility.
  - He described the complete series of capabilities under each core business area.
  - He reviewed aspects of the recommendations and BER's long-term vision "Characterize the variability's of biological systems throughout Earth and be able to understand and predict their rates of changes" and discussed how the new capabilities would contribute to that specific vision. Additional recommendations were also discussed.
- Advised that the draft plan would be refined through solicitation and incorporate the input from: a
  dedicated session JGI user meeting; BER June 2012 JGI Strategic Plan for Genome Sciences
  Workshop; JGI sponsored workshops; and a JGI website soliciting input.
- Described a nascent technology; high throughput design and construction of pathways and chromosomal size DNA at the JGI. He was asked why do this research at the JGI and noted that it was not the venue of private industry as it was too long-term, they wanted to develop it for DOE users, and the JGI maintains the sequence databases. Reviewed the long-term perspectives for 2016 through 2022.

### **COMMITTEE DISCUSSION**

Dr. Joachimiak noted that it was extremely important process that the JGI had undertaken in trying to predict the direction in which the JGI needed to go. He said that they had done tremendous work on providing data that was not available in other areas. He noted the complexity of genomics, from the sequence of genomes and elaborated and said in the next ten years a synthesis of everything was needed. Dr. Rubin said they have a niche and genomics is a big niche. He said there is KBase and their job is to try to help investigators synthesize bigger insights from mixing data. He said they were obtaining transcript-only data for all the organisms.

### **ENVIRONMENTAL MOLECULAR SCIENCES LABORATORY UPDATE**

### Dr. Allison A. Campbell, EMSL Director

Stated that she would be giving an update about what has been happening at EMSL over the past few years.

• Noted that considering the BER charge she was going to focus her talk around ideas, around how capabilities have advanced or can advance important programs.

- Described the presentation that would encompass: user statistics; science themes; science impact; thought provoking capabilities; and then review the results.
- Discussed the users of the EMSL and their locations nationally and internationally. Reviewed also the makeup of their users.
- Described several of their programs, the Wiley Visiting Scientists, Wiley Research Fellows and Wiley Postdoctoral Fellows.
- Described how science themes provide the framework for proposal calls and investments. Each theme of: Biological Interactions and Dynamics; Geochemistry, Biogeochemistry and Subsurface Science; and Science of Interfacial Phenomena was accompanied by a specific area of molecular research.
- Advised that their FY2013 proposal call would open from February 17<sup>th</sup> to April 2<sup>nd</sup>, 2012, and the proposals run for three years so if awarded users can get up to three years of access on the EMSL capabilities.
- Discussed some science research concerning systems-level dynamics of cyanobacteria under various environmental conditions. Noted the researchers as Lou Sherman (Purdue) and Himadri Pakrasi (Washington University of St. Louis).
- Discussed experiments being done at JBEI with microbial communities and switchgrass.
- Discussed some of the capabilities:
  - A mass microscope, C-60 ionization with the high spatial resolution of SIMS and high mass resolution of FTICR MS (Fourier transform ion cyclotron resonance mass spectrometry) with some illustrations.
  - Illustrations using micromodels.
  - Construction of a new \$8 million quiet wing allowing for new science opportunities such as 2 aberration corrected transmission electron microscopes, a helium ion microscope, 2 ultra high vacuum STMs (scanning tunneling microscope), TEM (transmission electron microscope)for biological samples and a dynamic TEM. Illustrations were discussed.
- Reviewed types of microscopy including high resolution, in situ, dynamic and high resolution, and dynamic. Illustrations were provided.
- Discussed the potential of time resolved in-situ ultrafast TEM (UTEM) and noted the importance if the researcher is interested in biology and chemistry as the processes can be viewed in real time.
- Discussed second-generation magnetic resonance spectrometry.

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- Described work being done at national laboratories in which they are thinking about building biosystems cartography at single cell and subcellular resolutions. Stated goals as: doing a census of cells from homogenous or mixed populations; at subcellular resolution, understand, model and manipulate populations of individual cells; and the acceleration of research in systems and synthetic biology for production of biofuels etc.
- Noted they are exploring the possibility of a compact X-ray light source at PNNL (Pacific Northwest National Laboratory)/EMSL or combining EMSL's expertise and capabilities with an in-house X-ray facility (like a Compact X-Ray Light Source CXLS) that would enable them to achieve an unprecedented level of multi-model characterization.
- Stated that with the new capabilities she thought that the community should come together and ask what science drivers that we should address and then what could these new types of ideas do. Added they have three workshop reports in draft that would soon go on their website.
- Discussed their recent triennial review that encompassed science, operations and management. Noted it was a positive review with five recommendations. Added that a plan of action and milestones would be submitted to BER.

### **COMMITTEE DISCUSSION**

Dr. Stacy asked about the ultrafast TEM, and its location. He asked how much of a leap forward was that technology? Dr. Campbell responded that going from one to two was doable. She said once that is up and demonstrated it would be an elite but not an insurmountable leap to go to the whole dynamics. She said it would come down to enhancing the laser systems. She confirmed that it was not a huge, insurmountable leap but definitely a challenge, adding a period of five to seven years.

Dr. Stacey referred the possibility of a connection between JGI and EMSL. He asked what had been happening in a concrete way to make the interaction between the laboratories take place. Dr. Campbell responded that it was happening on all levels. She confirmed that she and Dr. Rubin had discussed some of the things that they might be able to do and they had also talked with some of the PIs they have that might be interested in getting genomic data. She also said that in their science themes they were thinking about research campaigns for the future that would be larger teams. In connection with that discussion she said they had encouraged the PIs to reach out to the JGI and other facilities and they had done that. She thought that the power the SC has doing science across their user facilities is huge and under-tapped and she thought they should figure out ways to reach out.

A member referred to the methods for visualizing plant growth and movement and he asked whether they could think about a future in which they could bring the instruments to the field rather than the field to the instruments. He asked if that was on the radar. Dr. Campbell noted that they do that in a few areas in the climate area where they have mass spectrometers that they fly in planes and deploy out

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into the field. She acknowledged that some of the equipment was large. She acknowledged they had not thought about it but it was an excellent question.

### LUNCH

The Biological and Environmental Research Advisory Committee recessed for lunch for one hour.

### **KNOWLEDGEBASE DISCUSSION**

#### Dr. Adam P. Arkin, Physical Biosciences Division, Lawrence Berkeley National Laboratory

- Noted that they first started thinking about a resource like this in 2002 and they had proposed a
  national library of microbial ecology and physiology to rival the National Library of Medicine. Added
  that he would include microbial ecology and physiology and engineering at some point but at
  present they have a modest rendition but it is ambitious in its scope.
- Stated that they were a \$12.5 million a year project and their goal is to take the next step in the integration of biological data into enabling predictions of what biosystems do.
- Stated that KBase is serving the DOE mission which is to predict, control and design the biological components of energetic processes and environmental processes.
- Noted the challenge that was to deal with complex missions with rapidly expanding, intricately related diverse data types requiring a mean to augment scientists' ability to: filter information; focus attention; ask the right questions; and leverage other minds. Added that their idea was to create tools that would allow scientists to manipulate the data effectively.
- Described the ability of KBase to integrate science across activities, to manage huge amounts of data and information within individual activities and to integrate different activities or types of research.
- Stated that DOE had been instrumental in creating a large team to allow the science community to create all the data in a systemic way. Described the difficulties of numerous labs all working independently and treating data in individual ways but the DOE had standardized many of the practices.
- Outlined some of the components enabling the development of the Knowledgebase: the 2010 Knowledgebase R & D Project; the User Community Data and Resources; and University-Led Projects to Develop Computational Biology and Bioinformatic Methods.
- Noted that the DOE could not fund everything that needed to be done. Added their goal as software
  developers was to make an open piece of software, to lower the barriers to be able to develop code
  and deploy it in a way that everyone can use it, to be able to access data and to allow others to add
  on.

- Detailed the working goals of KBase as:
  - Knowledgebase enabling predictive systems biology.
  - Powerful modeling framework.
  - Community-driven, extensible and scalable open-source software and application system.
  - o Infrastructure for integration and reconciliation of algorithms and data sources.
  - Framework for standardization, search and association of data.
  - Resource to enable experimental design and interpretation of results.
- Explained differences between a database and a knowledgebase.
- Outlined their deliverable goals for 2013:
  - KBase infrastructure established in four laboratories including high-performance and cloud computing with routine 10+ Gb/s data transfer over ESNet between all KBase sites.
  - First public release includes: integration of data or reconstruct and predict metabolic and gene expression regulatory networks for up to 1,000 microbes to manipulate microbial function; and integration of phenotypic and experimental data for bioenergy plants to predict metabolic and regulatory genotypes enabling manipulation of biomass properties.
- Stated that to enable the DOE mission they were encompassing microbes, microbial communities and plants and they would begin to array information about these objects in the context of things like environmental transformation and energy capture.
- Discussed how they would target their activities.
- Stated that whatever analyses they do, they make the data available however the researcher would want. Stated that at Knowledgebase the tools they developed were about assigning measures of confidence and quality to everything so the researcher could be focused on what is important and where uncertainty lies.
- Stated that the microbes group is working on:
  - Reconstructing and predicting metabolic and gene expression regulatory networks to manipulate microbial function.
  - Increasing the capability of the scientific community to communicate and utilize their existing data.

- Enabling the planning of effective experiments and maximizing the understanding of microbial system function.
- Stated that the plants group is working on:
  - Deploying KBase capability that will allow for interactive, data-driven analysis and exploration across multiple-omics experiments.
  - Providing researchers in plant sciences access to comprehensive datasets from high-throughput experiments together with relevant analytical tools and resources.
  - Providing a platform for researchers to analyze their own experimental data and have results incorporated into the data exploration framework.
- Stated for the microbial communities group they have an overall goal of building a KBase metagenomic platform that provides:
  - Scalable, flexible analyses, link physiological and metadata sets to metagenomic sequences.
  - Data QC (Quality Control) and GSC (Genomics Standards Consortium)compliant data and standards for data collection.
  - Enable modeling of metabolic processes within a community.
  - Predict microbial growth in isolation and in a community.
- Described the infrastructure and what KBase is offering that includes: high speed data transfers; access to back end storage systems for large data sets; remote computer services for HPC (High Performance Computing), cluster and cloud based; workflow support; web UX access to data and computing; persistent and transient data management capabilities; and support for users, teams, projects and cross talk.
- Noted that KBase leverages ESNet for 10+ Gb/s data transfer between all nodes.
- Described the KBase cloud architecture and infrastructure and services.
- Stated that there were two ways to work with KBase:
  - Extend from below with additional core services that extend the KBase API (Applications Program Interface) and
  - Extend from above by plugging in applications that use the KBase API.
- Described a KBase user experience and how it would function.
- Listed what KBase would allow users to do:

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- Keep pace with the rate of data generation.
- Use interrelated data of different types.
- Develop analytical tools.
- Perform rapid comparisons across multiple genomes.
- o Allow free and open access to KBase data, models and simulations.
- Grow partners, developers, data generators or users.
- Coordinate with other researchers to target what experimental work is needed and to share results.
- Learn how to use KBase features of models and move into predictive systems biology.
- Noted their collaborators and presented an organizational chart. Described the different methods used by KBase to provide outreach to the community.
- Provided details of the KBase release/build timeline beginning in February 2012 to February 2013.

### **COMMITTEE DISCUSSION**

Dr. Stacey used an analogy of searching for information/data in encyclopedias and asked how it would work with KBase where they would see the unseen connections of models that would not at first be obvious. Dr. Arkin responded that that was what he meant by having the models. He said there were a couple of ways of looking at the problem. He used the same analogy advanced by Dr. Stacey and said that one would look for correlative inferences where you would make a correlation and you see there is a connection that you didn't think of before. He said what would make that useful because there are millions of correlative inferences and that you would get a confidence associated with it. He added where you can see that there are millions of pieces of data, over many replications that seem to imply a pattern, or a correlation that has a functional focus.

A member referred to the range of scales in KBase and he said modelers have problems when they try to transcend scale. He asked if he could give a ballpark for how many orders of magnitude differences in time constants or spatial dimension or time dimensions that KBase would swallow up. Dr. Arkin noted that he came from physical modeling background and that was a great question. He said most models that they would be talking about now would be statistical models where instead of there being a kinetic or diffusive process going on it would be more of an association and what you would get out of that would be probabilities and confidences. The member asked if there were constraints based on their standardization of data going into the database. He said it sounded like it is mostly DOE-connected data, it is not going out there and grabbing old data to bring in. Dr. Arkin responded that it was bringing in old data. He added that they had already built an ensemble interface, a geo-interface, an MTBI interface

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and noted that they were working with JBEI to figure out how to interface with them. He added that they would be building data loaders. Dr. Arkin said that DOE had led in ensuring that standard protocol and standard data is followed whereas when they do that for Geodatabase they have to discard for quality assessment reasons 60% of the database and the remainder would need warning flags due to missing or inaccurate data. The member noted that the commercial sector uses all data.

A member referred to security and asked if it was their vision that the KBase itself was also a database that would allow outside users, use existing data and test other hypotheses that someone was not working on. Dr. Arkin responded to the question of the use of all data out there and said it was probably a bad idea unless you use huge amounts of data and the bad data is washed out. He noted that the data they discard is data that is unintelligible otherwise they would assign a quality metric to it. Regarding security, he said that was about how you could own your data and he said they were working towards a good model for that where you can protect what you're doing. As to the question of whether KBase is a database he said the cost was high and they could not be a primary database for anything, they would always be a secondary database for other people.

A member identified herself as from the climate side of the committee and noted that their data was not in a good condition. She noted that they also have a large group of knowledge seekers. She added the atmospheric group was thinking about it for their ten-year plan but they are not even at first base yet compared to KBase. She wondered if there could be some cross-fertilization or how adaptable the kinds of things being done at KBase would be to the climate problem. Dr. Arkin responded that again, many of their problems or challenges resulted from the fact that they had real models to deal with and with measurements vast and small. He said it was inevitable they would come together and now was the time to be able to work and coordinate the groups together and to think of larger scaling where they would have to deal with real models.

### **BASIC ENERGY SCIENCES**

### Dr. Harriet Kung, Associate Director, Office of Basic Energy Sciences

- Thanked the committee for the opportunity of presenting.
- Noted that the program consisted of: materials sciences and engineering; chemical sciences, geosciences and energy biosciences; and was one of the nation's largest sponsors of a suite of scientific user facilities including X-ray sources, neutron sources and nanoscale science research centers.
- Stated the basic energy sciences portfolio aims to understand how nature works, to predict and ultimately control matter and energy flow at the electronic, atomic and molecular levels.
- Described some of their challenges as:
  - Synthesize new forms of matter.

- Direct and control matter and energy across multiple length and time scales.
- Explore materials and chemical functionalities and their connections to their structure and composition.
- Applying the basic research knowledge to transform energy applications and technologies.
- Noted that BES has engaged the community in helping them with strategic planning activities and these fall mainly into three categories: science for discovery; science for national needs; tools.
- Described several examples of strategic planning that BES and their advisory committee had done and this concerned the BESAC Grand Challenge Report.
- Continued to discuss the Grand Challenge Report and in relation to it they had asked what were the five intellectual drivers that inspire the community and the results were:
  - The report presented an opportunity to transition from the 20th century of observation science to the new opportunities of the 21st century in terms of control science or how do we control matter and energy down to the atomic molecular scales.
  - Control the quantum behavior of electrons in materials.
  - Synthesize atom by atom new forms of matter with tailored properties.
  - Control emergent properties that arise from the complex correlations of atomic and electronic constituents.
  - Synthesize man-made nanoscale objects with capabilities rivaling those of living things.
  - Control matter very far away from equilibrium.
- Described the BES Basic Research Needs Reports started in 2002 which were workshop reports and was a first attempt to do road-mapping for basic research.
- Discussed a chart relating to sustainable energy and high technological materials and chemistry. It concerned the transition of the current way of viewing and utilizing energy where essentially the resources are used as commodities and then the use of the commodities by conversion or combustion. Stated by contrast the future and sustainable energy requires that they design a powerful and diverse functionality from the limited materials in chemistry. Added that the way that these resources are converted has to be more efficient, so direct conversion of energy whether it would be solar, wind or ocean.
- Described how the discovery process has been transformed over the past two decades by the development of powerful research centers including: world-leading x-ray and neutron sources; nanoscale science centers; and high performance computing. Added that they are able to

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synthesize, characterize and model materials and chemical behavior at the length scale where this behavior is controlled.

- Commented on the three types of funding modalities as: core research with PIs and small groups;
   \$2-5 million Energy Frontier Research Centers with multi-investigational and multi-disciplinary centers; and \$25 million Energy Innovation Hubs with large research centers focus on co-locating and integrating multi-components and multi-disciplinary research.
- Noted that there are 46 EFRCs in 35 states, these were launched in 2009 for different types of fuels and some concerning energy conversion and energy storage. Reviewed details on the centers' reviews and management of the EFRCs.
- Discussed JCAP (Joint Center for Artificial Photosynthesis) as a solar fuels integrated hub funded at \$20 million a year and some of the research goals.
- Described some of the basic research projects that include:
  - How an inexpensive solar cell absorbs nearly all available light fundamental research to rooftop applications. Researchers from different universities are collaborating with each other in this research. A small start-up company began as a result of the research funded out of the DOE technology program and is a successful R&D integration with the basic research components supported by the SC and the technology programs supported by EERE. The British company, BP has given additional funding to further develop the technologies.
  - Research concerning superplastic forming was described reducing vehicle weight, improving fuel economy and reducing emissions. The basic science concerns mechanistic understanding of the aluminum alloy microstructure and the superplastic deformation. The R& D was described and it was noted that the technology was further developed by General Motors.
- Stated she would discuss tools that had often helped to create partnerships between BER and BES:
  - The X-ray synchrotron light sources that has had significant growth in the user base since its inception because of use by life scientists as well as geoscientists and ecologists.
  - The LCLS, X-ray laser is new with 2011 as the first year of full operations for the Linac coherent light source at SLAC National Accelerator Laboratory. Topics being studied are hollow atoms and the structure of biomolecules.
- Discussed three neutron scattering facilities: The Spallation Neutron Source (SNS); The High Flux Isotope Reactor (HFIR); and The Lujan Center.
- Noted that BES user facilities served over 14,000 users including over 300 companies including 30 Fortune 500 companies.

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- Stated that three Nobel Prizes over six years had been won using X-ray crystallography by Roderick MacKinnon in 2003, Roger Komberg in 2006 and Venkatraman Ramakrishnan, Thomas Steltz and Ada Yonath in 2009.
- Described the BES FY 2013 budget and noted a large fraction went toward facilities.
- Commented on several facilities she hoped would have more engagement with BER and the BER community and one is the NSLS II (National Synchrotron Light Source) that is on a fast track being completed hopefully by the late 2014/early 2015 timeframe. Noted it was a highly optimized X-ray synchrotron with exceptional brightness and beam stability and a suite of advanced instruments.
- Describe three further facilities in which they were maintaining world leadership in light sources: the Linac Coherent Light Source II; the Advanced Photon Source Upgrade and the NSLS-II Experiment Tools. Noted that these upgrades were in response to competition around the world including Germany and Japan.

### **COMMITTEE DISCUSSION**

A member asked how she would control emergent and subemergent properties that are usually considered unknowns or unknowable. Dr. Kung responded that it was her sense he was asking about the LCLS front. She responded that proof of principle was important and she said that what she meant to mention is that what they have done is use molecules with known structure and composition and try to see whether they can actually alter that in any way. She said one of the recent experiences she had at LCLS was that they were testing photosystem two with a structure not as well known as photosystem one. She added that what they had done to ensure that what they had observed was the virgin property was they added a spectrometer in addition to the defractometer. She added that in addition to capturing the defraction data they were also capturing the chemistry, the spectrometry of the same particle.

A member referred to the 3-D elemental mapping as she thought there might be a potential application to the phenotyping that needed to be done for microbes. She noted that the presentation included trace elements for the mapping and asked could that be a higher throughput and also, could they also look at more abundant elements like carbon, hydrogen and oxygen. Dr. Kung responded that the throughput is definitely something that they were focusing on not only for BER experiments but also for a lot of industry usage. She added that high throughput was one key requirement so they were focusing on designing and adding high throughput whether through robotics or other types of accessories to help the throughput issue. She said it was her understanding that it was done through florescent tomography that might be a slower technique. Dr. Steve Dierker added that there had been some work using soft X-rays that would be able to access the lighter elements and doing tomography work.

A member complimented BES on doing an incredible job maintaining the facilities. A member indicated that he was pleased there was a significant investment in NSLS-II and APS-U. He asked if they could

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consider for the future investing in detectors, optics insertion devices that match into the source. He thought the current detectors were too slow. Dr. Kung stated that they had also come to the same conclusion. She added they were thinking about doing a workshop on detector research needs and noted that that would be an area where they could solicit input.

A member referred to the operation of the JCAP and how that works as a hub. She asked if independent scientists would exchange information and if that would eliminate competition. Dr. Kung said as far as operation was concerned JCAP had two main hubs, one JCAP North located at Berkeley and JCAP South located at CalTech in Pasadena, California and both use modern-day telecommunications for routine communication. She explained they did have co-location of talents at the two main sites. She added that referring to competition and said of course, there would be competition but also noted that there were many opportunities for collaboration with the sharing of materials and databases. She stated that scientists would always compete but the spirit of the hub was to coordinate the information exchange and facilitating more collaboration was what JCAP was about.

Dr. Stacey referred to BESAC and asked about her perspective as AD of BES, her feeling about how she interacted with BESAC and what they did well. He asked if she had any advice for how they could improve BERAC. Dr. Kung responded that she was pleased to hear the praise for BESAC but said she could not take the credit. She noted that Dr. Dehmer had established the BESAC model and said that Dr. Stacey might want to contact Dr. John Hemminger, the BESAC Chair. She said her observation was that the committee takes a forward-looking view in terms of setting the whole community's vision and this was reflected in its use of improvements to basic science and road mapping. She mentioned also the second wave of the Grand Science Challenges Workshop Report, again a trend-setting workshop and she thought it anticipated the future excitement but also reflected that in the context of a science agency mission need.

### **BREAK**

The Biological and Environmental Research Committee recessed for 15 minutes.

## CONTINUED DISCUSSION OF CHARGE: TECHNOLOGY IMPLEMENTATION FOR LONG TERM VISION

Dr. Stacey commented that he had been told that the Grand Challenge Report that BERAC had generated was submitted to the Society for Technical Communications and was judged as "Distinguished", the highest rating and because of that rating was automatically entered into the international competition. He commended all that were behind the report.

Dr. Stacey reminded members that there was a sub-committee put together at the last BERAC meeting. He noted that there were conference calls and they also sought input from other committee members. He said the draft that all members had received reflected the discussions. He stated that one of the things they needed to do was to think when the report should be finalized. He said that the original plan

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when they had two annual meetings was to discuss it at the February meeting, continue work on it and have a final copy ready for the fall BERAC meeting where it could be voted on and sent to Dr. Brinkman. He said as they were now having a meeting in June and so he said other than the content they needed to decide whether they could finalize it by the June meeting.

Dr. Stacey asked if anyone wanted to make any edits or suggestions and especially reached out to the new members.

A member noted that after reading it she felt that the four general themes were the right themes. She added that the biological content elicited excitement but that the section on climate/environmental content did not seem inspiring. She added that it didn't seem that there was the same level of vision, a bit of business as usual and she felt that it did not reflect the balance of the committee. She thought the information piece was the most important piece but also lacked the high interest level of the biological content. She thought the field measurements with the ARM information were repetitive and the content did not appear challenging in a new way, in other words, it lacked a new vision.

A member noted that it was a small group that reached out to focus groups to get ideas and she thought one thing that they should decide was are these the right four categories. She added that what was written did not appear to go very deep. She noted that it was difficult to go deeply into topics when there were not driving science questions or some sub-questions that are topical to aerosols and clouds or carbon in the soils for example. She said the ideas to think about are do they have the right structure and then when it is established that they do, then dig in deeper and talk about each category. She also said the strength would be in bringing the four tools together to tackle a question. She thought the ideas were there, but not deep and not integrated yet.

Dr. Stacey said the structure was up to them and that could be changed. He said they wanted to be forward-looking and were looking at, at least a decade forward with the report. He referred to the report that they have and noted that one of the ways they dealt with the general idea versus the specific idea is to put in boxes where you might have a specific example. He said this could be used to integrate the text or ask a specific question or give examples.

A member said that for the climate issues they have the right things in there but perhaps not in the right way or distribution. He added what would make it transformational is to actually turn what they have or what they will have into knowledge by having a KBase applied to the climate problem. Dr. Stacey said to put it into perspective as a biologist he noted that they were a long way from taking information and turning it into new knowledge.

A member noted in the first section and points dealing with integrated networks he thought the DOE had a problem in their past performance to the solution of that problem. He said that the NSF was building big networks built on the premise that if they build them they will find out something. He thought the DOE was good in large-scale experiments with focus on questions. He made another point about simulation and analysis frameworks and said there are some fundamental questions that are

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relatively untouched. Dr. Stacey asked if he was saying that he was trying to understand how carbon uptake translates into growth. He asked if that was his question. The member responded that the answer of how much carbon is being stored when he has a leaf area of five is not knowable unless one would constrain it by understanding more about the mechanisms and he elaborated.

A member referred to the parts about the observation networks and he noted that there are different networks for different questions. He said there was a lot of popularity among the climate community in doing data simulation and in that case they would need a dense network with a lot of cheaper sites. He said there are also a lot of models that are very mechanistic and they would need detailed sites with lots of metadata and ancillary measurements that are more expensive. He said getting back to thinking of developing a system that is science-based you would then design and fund the appropriate types of networks for the types of questions and be more targeted. Dr. Stacey asked how that would be turned into a recommendation. He said it was factual but where is the recommendation? He said it needed to be turned into a recommendation about what is the best priority in the next decade. The member said he was a fan of model hierarchy approaches. He said what was needed was a hierarchy of simple models, the most complex models and under some situations a simpler engineering model to do applied work. He added that conversely they needed very detailed mechanistic models to understand how the system is working. He added that they needed to have a multi-faceted approach in terms of theory, model and observation.

A member said that she wanted to see the office not shy away from production agriculture as well. She thought that many of the tools discussed at the meeting could be really helpful to the modeling efforts and the predictive modeling work in production agriculture. She referred to the research coming out from work on the genome of standardization and transparency of assumptions and a requirement of doing that to obtain grants or be a part of the database is necessary on the lifecycle analysis work and the land use change work. She said the Argonne National Laboratory and Oak Ridge National Laboratory had done a great job with those efforts. Dr. Stacey noted that there were approximately 26 long-term ecological research sites and only 1 devoted to crop production.

A member mentioned that he would not necessarily continue the former member's comment from an agricultural crop production but more biomass production. He said a long-term view of what they were trying to accomplish would ultimately be replacement feedstock for hydrocarbon fossil fuel-based materials, fiber and other kinds of energy sources, ecosystem restoration of carbon storage, so more a biomass optimization than just a crop production issue.

Dr. P. Robertson said that he wanted to speak about the value of keeping observatories as one of the four pillars of the report. He thought it was a very important concept, scaling across the boundaries, physical boundaries, soil, plant, atmosphere, microbes etc. as well as disciplinary, genomic, biogeochemistry and atmospheric sciences. He thought they should be careful in identifying what BER could bring to the effort that would be unique to BER and differed from and complemented existing efforts, especially NSF efforts. He noted that BER provided advanced instrumentation that was directed

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toward specific fundamental questions. He added another was the modeling capacities and cyber infrastructure and environmental data handling and curating was a further specialized area that BER could contribute.

A member said that some of the strengths of BER he would think of would be trace gas cycles, things related to carbon, water cycles and modeling and climate. He said one of the arguments for NGEE was that you needed to have an observatory or footprint that was large enough that you could model it at the global scale. He thought other networks were not thinking about is how to take those processes and put them into a bigger scale. He suggested having a set of networks that were relevant to answering global questions relating to carbon, water cycles and climate that might be an appropriate way to think about that.

Dr. Stacey said one of his concerns was to think about the logistics and he noted that they had had a lot of good discussion, both general and detailed, but they would need to capture that in the document. He said he did not have all the knowledge and did not have the time to edit such a document so it would fall to someone else. He agreed with earlier comments that they needed some very forward-looking specifics. He gave as an example Dr. Campbell's presentation in which she stated that she had three specific instruments that she would like to develop over the next 5-10 year period. He said he was not necessarily agreeing with her suggestions but emphasized that any three specific kinds of examples could be woven into the document in response to specific biological questions. So he asked how they would capture the information in a mechanistic way, secondly what were the kinds of specifics that were needed and three, if boxes were going to be used, what the biological questions would be.

A member suggested as a question, the photosynthesis allocation problem and another one, the scale problem.

A member suggested that if they were thinking of the long term they should look at the report to determine what data was missing or needed and then consider what tools and databases would be needed to support the vision. He said that they would need to synthesize all the data that would be coming in to improve their models.

Dr. Stacey commented that they were told that the report was not meant to be a strategic plan, not a roadmap. He said he had received some criticism that it had been difficult to find actionable items or once the report is read, how would one turn those recommendations into action. Dr. Stacey said that his sense is what they wanted out of their current charge was actionable items. He stated that they wanted BERAC to give priorities on things that they could turn into action.

A member said he felt that the first actionable item should be in climate science that they should have some facility for turning data into knowledge. He said ARM had been instrumental in generating important data but much less successful in turning the data into something that could improve models that was its stated objective.

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Dr. Stacey noted the climate group was having problems with data integration and suggested bringing in groups from other areas that had more funding, such as scientists working on medical research, and sharing their knowledge in the form of a workshop. He thought it might be a good idea to suggest this to Dr. Brinkman rather than having these types of ideas come down from the Office of Science and he asked for any comments.

A member thought that cross-fertilization of that nature was very valuable. He thought that at times certain fields were in a type of limbo and that external ideas could be very helpful.

A member thought that it was a very useful role for BERAC to be in leadership for the community as Dr. Stacey had given as an example, the role that BES was taking.

Dr. Stacey asked Dr. Julie Carruthers to speak about the Graduate Fellowships as a question had been raised and she had pulled together some facts and figures.

### SC GRADUATE FELLOWSHIP PROGRAM

Dr. Carruthers explained that the SC had received input from the scientific community through COVs (Committees of Visitors), workshop reports, external studies from the national academies regarding the need to support scientists in the early stages of their careers. She stated that when the America COMPETES Act (America Creating Opportunities to Meaningfully Promote Excellence in Technology) was passed in 2007 and 2010 it authorized graduate fellowships for the DOE and early career research programs for the SC. She added that when the Recovery Act was passed it presented an opportunity of them to initiate two programs to address workforce development needs, one was the Early Career Program and the other was the SC Graduate Fellowship Program. She stated that the award is a three-year graduate fellowship and the support is \$35,000 per year for a living stipend, \$10,500 per year as support for tuition and \$5,000 a year research stipend. She added that the program has a required annual meeting of all the fellows taking place in different DOE labs each year where they can share research results and meet fellow scientists. They get tours of the scientific user facilities and can participate in professional development sessions.

For eligibility they must be U.S. citizens and can be a senior undergraduate or a first-year graduate student at the time of application or not currently a student but enrolled in a qualified PhD program at the beginning of the fellowship year. One of the requirements is that they pursue an area of graduate studies that is aligned with an SC research program area. She reviewed the application process and provided additional details using the Graduate Fellowship Program website (<u>http://scgf.orau.gov/</u>). She commented that the current controversy regarding the program was a philosophical belief that the NSF rather than the science mission agencies should be the main supporter of graduate fellowships in the science area. She noted that they have been asked in the FY2012 appropriations language to write a report on what their ten-year plan is for the program and what is distinct about the program from the NSF from the graduate fellowships and they are in the process of doing that. She was asked how many applications were received for the current year and advised it was 1,400 now under review.

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### **PUBLIC COMMENT**

There was no public comment.

#### ADJOURNMENT

The Biological and Environment Research Advisory Committee adjourned for the day at 5:30 p.m. The Committee will reconvene tomorrow, Friday, February 17, 2012 at 8:30 a.m.

### FRIDAY, FEBRUARY 17, 2012

### **CLIMATE AND ENVIRONMENTAL SCIENCES DIVISION UPDATE**

#### Dr. Gary Geernaert, Director

- Stated that the highlights presented for his division included input from everyone.
- Commented on some of the key points that he had emphasized during the October 2011 BERAC meeting:
  - An agreement in the division that their mission focuses exclusively on system predictability which is what kind of certainty can they make of statements in the future using model-based or community systems and where the gaps are to help guide future investments.
  - A set of goals were developed to further their strategic planning.
  - The USGCRP is a serious priority and the inter-agency coordination body in Washington of the federal agencies. DOE is one of the primary agencies. Some of the other dominant agencies are NSF, NOAA (National Oceanic and Atmospheric Administration) and. BER wants to ensure that their strategic planning process overlays with what the USGCRP is doing.
  - The establishment of linkages to DOE applied offices.
  - A concerted effort was made to get a significant presence at the scientific societies and through town hall meetings.
  - An emphasis on visionary science, a uniqueness and value.
- Provided the current CESD mission statement: "To advance a robust predictive understanding of Earth's climate and environmental systems and to inform the development of sustainable solution to the Nation's energy and environmental challenges".

- Noted that an effort was made to emphasize the concept of predictive understanding that would unify all the programs.
- Gave the five strategic goals set out by the CESD:
  - Synthesize new process knowledge and innovative computational methods advancing next generation, integrated models of the human earth system.
  - Develop, test and simulate process-level understanding of atmospheric systems and terrestrial ecosystems extending from bedrock to the top of the vegetative canopy.
  - Advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable systems level prediction and control.
  - Enhance the unique capabilities and impacts of the ARM and EMSL scientific user facilities and other BER community resources to advance the frontiers of climate and environment science.
  - Identify and address science gaps that limit translation of CESD fundamental science into solutions for DOE's most pressing energy and environmental challenges.
- Reviewed three platforms to integrate the science and identified them as observational infrastructure, community data infrastructure and community models.
- Discussed the NGEE concept and noted that the "Next" refers to target systems that are globally important in climatically sensitive regions and that have been relatively unstudied. Stated that the work would be deep experimental work but also have a strong modeling overlay so a bridge between modeling and experiment. Stated they were looking at how the NGEE paradigms might be used to advance the community Earth System Model (ESM) or any community model.
- Noted that the NGEE concept would be extending beyond the Arctic to include a Tropics NGEE starting in FY2013. The location will be determined through input from a future workshop.
- Provided some management updates including federal collaborations in the form of participation or discussions and with the DOE and many other agencies. Added that for some agencies they were trying to develop some collaborative or coordination arrangements.
- Detailed management updates on town halls at scientific societies including the Ecological Society of America, the American Geophysical Union and the American Meteorological Society and stated that they had advertised some of their activities in the scientific societies to get more of an outreach presence and obtain input from the community.
- Continued to detail updates and stated that in the pipeline there was the question of what the strategy should be for the seamless community earth system prediction. Noted that earth system prediction started at the decadal scale and going into the future.

- Reviewed programmatic activities:
  - Some reviews are completed. The EMSL review was in its last stages and the LANL SFA (Scientific Focus Area) review that took place in July 2011 was also in last stages.
  - Upcoming reviews in FY2012 were listed.
  - Upcoming PI meetings.
  - Upcoming workshops including a root modeling workshop on March 7-9 which is new for the division. A TES Experiment-model fusion workshop on March 19-21. Two workshops in the pipeline are the water cycle and the NGEE tropics.
  - Research opportunities were listed including: ARM 16 preproposals; TES panels met in January and 141 proposals were reviewed; Early Career proposals; SciDAC 6 proposals were reviewed; and Ameriflux 6 white papers were received.
- Reviewed some changes in the budget for FY 2012 and FY 2013.
  - The changes in the budget investment were driven by the strategic directions that the division was taking.
  - Stated that for the ARM program two new facilities were established, a permanent site facility in the Azores and a longer-term mobile facility based in Alaska.
  - There is also growth in the areas of UQ (Uncertainty Quantification) and diagnostics.
  - A last area of growth is climate sensitive geographics including the Arctic and the Amazon.
  - The decline in the budget concerned the subsurface program. He said that in light of that development they were making an effort to build up other portfolios in the soil system regime such as root and permafrost systems.
- Discussed the ARM climate research facility and noted it had gone through a major transformation
  with ARRA (American Recovery and Reinvestment Act of 2009) funding. Noted that the funding had
  a dual benefit putting radar and LIDAR systems onto ARM sites to expand coverage in three
  dimensions, cloud, and aerosol and precipitation characteristics. Added the other benefit was that
  the scale of a ten by ten kilometer domain that the ARM facilities were able to examine it would
  approach the scale the next generation community earth system models.
- Described the two tropical studies underway, one would be NGEE Tropics yet to be defined and the GOAmazon ARM experiment in 2014. Added that the GoAmazon was a major campaign looking at the impact of biogenic aerosols, rain forest and pollution on clouds.
- Reviewed some of their science highlights:

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- Greenland ice sheet modeling group and Los Alamos was a key player. It involved building dynamical models of Greenland and Antarctica and is critical to the process. The study summarized work that took place where they analyzed a decade of observations in Greenland at three glaciers.
- The second highlight focused on the near-surface permafrost in the NGEE Arctic effort.
- The third highlight is looking at global models and validating them against some observations, re-analyses as a critical piece of how they extend the community earth systems capabilities.
   Discussed the motivation, approach and results.
- Discussed the demise of Arctic clouds due to ice crystals. Noted the goal as an understanding of the formation and dissipation of Arctic clouds needed for global climate models. The approach, results and impact was reviewed.
- Discussed ARM data and models in connection with ice crystals in clouds in the tropical cloud systems.
- Discussed the growth and expansion of boreal shrubs in relation to warming. Noted the objective was asking how does the shrub height and expansion affect boreal climate and permafrost? Reviewed the approach and results.
- Discussed high performance computing simulation of complex subsurface processes. The objective was to simulate the coupled physical, geochemical and microbiological processes controlling uranium mobility during an in situ bioremediation test. The new science and significance was discussed.
- Commented that during the next six to twelve months they would be moving their strategy forward and adding onto the five goals previously noted, detailed objectives, narrowed so that they have a sufficient investment to make a difference. Added they want to make the investment unique to the DOE but extend their collaboration to the right agencies.

### **COMMITTEE DISCUSSION**

A member referred to the last comment and said it was a bit ambiguous. He asked if he could elaborate and in particular what he would give up in the research program. He also noted that they were taking some steps away from basic research in the subsurface science program. He asked where he thought things would be in the next couple of years. Dr. Geernaert responded in two parts, first the DOE-wide answer and then the division answer. He said for DOE they looked at the biggest impact on DOE in the long term in a holistic sense so when there are decisions made on what areas to grow or what areas to shrink or redirect, it would be based on a higher-level discussion on where is DOE broadly heading. He said from the perspective of the division they tried to look out to the future and looked back to ask what were the really bold cutting areas that they needed to invest in and how should they be realigning the

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portfolio in the right way to achieve those ends. He said they were trying to respond to a number of fingerprints on what the priorities should be and at the same time invest in areas where they are going to have significant growth.

A member referred to the NGEE and noted he was involved in some workshops on planning and at that stage they were viewed as a user facility for scientists to go and do work. He asked if that was still the case. Dr. Geernaert responded that he would not call them user facilities but they would be sites collecting data for the research community to have access to. A member asked if the NGEEs would have experimental components to them. Dr. Geernaert responded that they were in large part dominated by experimental components. The member asked if the research community had input into those experimental components. Dr. Geernaert said yes they did.

A member referred to the document for grand challenges and then the long-term vision. He asked if he saw the new strategic planning like implementation or a new initiative in the context of new information. Dr. Geernaert responded that it was almost an implementation of the long-term plan and noted that everything conformed to that.

A member referred to work that could go on with inter-agencies and asked him to comment. Dr. Geernaert responded that they were working heavily in engaging with other agencies and he gave several examples including work he was currently doing with the USGCRP.

### **SCIENCE TALK - WHAT CAN WE LEARN FROM CLIMATE MODELS?**

#### Dr. Judith Curry, BERAC Member and Georgia Institute of Technology

- Commented that she was invited to give a science talk and discuss her own personal research but decided to give more of an applied philosophy of science presentation related to climate modeling.
- Stated she was not a member of any of the model development groups. Added that she uses climate models and her research has contributed to some of the parameterization developments in cloud physics and sea ice.
- Noted that her perspective on the topic comes from her engagement with a broad range of people external to the climate science community including blogging activities. Added she had engaged with PhDs in physics, nonlinear dynamics, nuclear engineering, aerospace engineering and many of those people are unconvinced by what she is doing with climate modeling.
- Thought that some of these groups had some valid points so noted that she believes they have to think outside of their own community.
- Stated that she was trying to look at the bigger picture and would look at two themes: Dr. Geernaert's theme of uncertainty and confidence; and the second theme is: where would the new ideas come from.

- Noted the DOE Climate Change Research Program and its strategic plan for 2009 that included the
  comment that climate change research had moved from determining if Earth's climate was changing
  to trying to understand how quickly it is changing, where the changes will occur and what the
  impacts are. Stated that climate models were the best available tool but they still have some
  weaknesses. Also stated was the fact that projections of future climate change were the basis of
  national and international policies concerning greenhouse gases.
- Reviewed the strengths and weaknesses of climate models described in a report from 2008.
- Described the current path for climate modeling as:
  - Increasing resolution and adding complexity.
  - Fully interactive earth system models (chemical, biogeochemical, land cryosphere); interface with human systems models.
  - Seamless prediction across timescales; data assimilation and initialization.
  - Downscaling for regional applications.
  - Infrastructure.
  - Communication of climate model results (including uncertainty, credibility); engagement with stakeholders; usefulness for decision making.
- Provided a quote from the journal Studies in History and Philosophy of Modern Physics, and an article called: "Modeling and Simulation in the Atmospheric and Climate Sciences" that raised multiple questions about the use of models by researchers including the many uncertainties and scientific gaps in the creation and use of their model constructions.
- Reviewed what makes up belief and confidence in climate models using the formal and informal approaches. Stated the informal approach used by GCMs (General Circulation Models) that has dominated.
- Stated why researchers have confidence in their models and stated that it derives from:
  - The theoretical physical basis of the models.
  - The ability of the models to reproduce the observed mean state and some elements of variability.
  - Some successes of numerical weather prediction.
  - The term "comfort" and what it means to model developers.

- Detailed some of the issues causing rising discomfort that other researchers outside the climate community have with the development of current models.
- Addressed these issues and discussed verification and validation including a definition as follows: The process of checking and documenting that a model is built correctly and meets specifications and is an accurate representation of the real world from the perspective of the intended uses of the model.
- Reviewed the arguments for and against the verification and validation of GCMs. Described secondly the verification and validation of scientific models and reviewed the recommendations.
- Described the validation of GCMs as given in a paper by Pope and Davies (2011) on the Testing and Evaluating of Climate Models.
- Commented on and described some climate model applications from the perspectives of pure science, the IPCC and policy.
- Discussed the scientific understanding of the climate system noting the GCM challenges and other approaches.
- Discussed the IPCC issues: the attribution of past climate variability and change; simulation of plausible future states; and support for emissions reduction policies. Reviewed the challenges and other approaches.
- Discussed the total solar irradiance measurements from space and the three different total solar irradiance measurement composites.
- Discussed the two main solar reconstructions, one shows no trend over the last couple of centuries and the other shows an increase in the earlier part of the 20th century and noted that this showed the uncertainties not being accounted for in the attribution studies.
- Discussed projections of future regional climate variation for use in model-based decision support systems and described the GCM challenges and other approaches.
- Reviewed the prediction and attribution of extreme weather events and indicated the challenges including the fact that models do not currently predict explicitly the many types of extreme weather and the fact that much higher resolution climate models with much larger ensemble sizes are necessary. Discussed other approaches in addition.
- Described the projections with regard to future risks of black swans and dragon kings. Noted the GCM challenges which stated that: GCMs are currently incapable of predicting emergent phenomena and asked would more complex or higher resolution GCMs be able to generate

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counterintuitive, unexpected surprises. Stated other approaches including synchronization in spatiotemporal chaos or theoretical developments from nonlinear dynamics or network theory.

- Stated that they needed a plurality of models developed and utilized in different ways for different purposes.
- Asked and discussed whether GCMs are especially policy useful. Gave several advantages of the models and disadvantages.
- Stated that she wanted to see fields external to BER contribute to the design of models and some included: solar physics, nonlinear dynamics, statistics, engineering regulatory science, network theory and information theory. She thought perhaps researchers at LANL (Los Alamos National Laboratory)and COSIM (Climate, Ocean and Sea Ice Modeling) were working on some new models.
- Discussed the understanding and representing uncertainty in models and reviewed some of the challenges and other approaches.

### **COMMITTEE DISCUSSION**

A member noted he had similar experiences with NCAR about 15 years ago. He asked if she had outlined a plan for an alternative for DOE. He said he agreed with the idea of getting back to basic science and he noted a lot of resources were going into production runs. He asked if there was a niche for the DOE to get back to science and use some of her suggestions. Dr. Curry said she hoped so.

A member referred to her point of whether GCMs or models are fit for use. She said she thought it was a valid question but she said they also need to ask how the models were being used. She said both sides were important so a lot of communication needed to be done in order to communicate what could be provided and how it could be used. For her second comment she referred to the validation. She noted that for climate models in many different levels they had done many different types of validation. Dr. Curry agreed and said that the issue was getting it into a document and a systematic thing that somebody external can look at and make sense of it and decide whether or not to have confidence in it.

A member said in support of some of her points he was making two points. He had published a paper in 2008 using about 10-20,000 hours of ARM data to parameterize ice crystal false feed that he noted was an important issue in GCMs. He said the people at GFDL wanted to use the parameterization but they had to freeze their model in 2009 to do their runs. He said also that he would be very interested to have an external entity evaluate the approach that he was taking to understand feedback in the models because you would have extraordinarily complicated nonlinear models and feedback that would be driving the analysis of cloud feedback for instance that was in turn driving the entire modeling community in one direction or another. Dr. Curry noted that that had been discussed on her blog.

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### **BREAK**

The Biological and Environmental Research Committee recessed for 15 minutes.

### **BIOLOGICAL SYSTEMS SCIENCE DIVISION UPDATE**

#### Dr. Susan Gregurick, Acting Division Director, Biological Systems Science Division

- Thanked all the members of BERAC for the opportunity to come and brief everyone on the activities that BSSD has undertaken.
- Took the opportunity to also thank her colleagues in BSSD for their support and active involvement in the program over the last four months. Noted it had been a great learning experience.
- Reviewed their completed programmatic activities:
  - The findings and recommendations from the reviews of the three Bioenergy Research Centers have gone out to the Center directors and the responses are expected shortly.
  - A Joint Genome Institute review was completed.
  - A Biosystems Design Workshop took place in July 2011 and the findings are available on the web (<u>http://genomicscience.energy.gov/biosystemsdesign/index.shtml</u>). Copies of the executive summary are available at this meeting.
  - A Report from the Switchgrass Research Group is available on the web (<u>http://genomicscience.energy.gov/pubs/switchgrassreport.pdf</u>).
  - Annual Principal Investigators Meeting of the USDA-DOE Plant Feedstocks Genomics for Bioenergy took place in January 2012.
- Reviewed their ongoing programmatic activities:
  - Genomic Science Principal Investigator's Meeting on February 26-29, 2012.
  - Open solicitations including the joint DOE-USDA Plant Feedstock Genomics Notice;
     Integrated Nuclear Medicine Research and Training Projects of Excellence; and Genomic Science: Biosystems Design to Enable Next-Generation Biofuels.
- Discussed the Biosystems Design initiative and stated it was research to establish biological design rules that would enable the predictive design of innovative natural and hybrid systems for clean energy production. Stated that they were interested in the discovery and synthetic redesign of plant and microbial systems that would push the science frontiers and pave the way for sustainable production of advanced biofuels and bioproducts. Stated that to achieve this they needed to have a research focus:

- A synthesis of new synthetic biology methods.
- New genetic toolkits.
- Predictive integration of components and processes.
- Stated characterization and testing that would:
  - Verify and validate computer-aided design toolkits.
  - New testbeds to prototype performance and function.
- Provided details of a new funding opportunity announcement, the Biosystems Design to Enable Next-Generation Biofuels in two lanes:
  - Microbial systems design for biofuels.
  - Plant systems design for bioenergy.
- Stated that for microbial systems design they want to develop new modeling algorithms, innovative biodesign technologies, to define, build and test functional biological modules for the generation of novel biological systems that advance toward the production of biofuels.
- Stated that for plant systems design for bioenergy they wanted to develop new technologies to redesign bioenergy crops that can grow in marginal environments while producing a high yield of biomass that can be easily converted to biofuels.
- Reviewed upcoming programmatic activities:
  - Several reviews including a Human Subjects Protection Program reviews and Scientific Focus Areas among others.
  - Symposia and conferences three upcoming conferences are being held.
  - A JGI Strategic Planning for Genomic Sciences Invitational Workshop
- Described the BSSD response to the Committee of Visitors from June 2011. Detailed the COV recommendations and appropriate action plan and noted the full details are on the web (http://science.energy.gov/~/media/ber/berac/pdf/BSSD\_COV\_2011\_response.pdf).
- Commented on some of the research being done at BESC (Bioenergy Science Center) concerning the design of low lignin, high biomass yielding plants. Commented on the objective, approach and results/impacts.
- Described research being done at JBEI concerning microbial conversion of switchgrass to multiple drop-in biofuels and noted the objective, approach and results/impacts.

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- Commented on research being done on using omics to understand impacts of soil warming on microbial carbon and nitrogen cycling and noted the objective, approach and results/impacts.
- Described research concerning plant feedstocks and the research concerned maize juvenility gene enhances biofuel production in bioenergy crops.
- Detailed research from the low dose research program and more particularly understanding DNA repair center formation is greater at lower does than at higher doses.
- Commented on some of the latest news out of JGI and their latest collaborations and some selected JGI high impact publications.

### **COMMISSION DISCUSSION**

A member referred to the SFAs and asked about the development and oversight of those. He noted that the response was that they would have reports. He asked about the SFA reviews and asked if they were as engaging as the BRCs. He also asked how SFAs are developed, were they aligning with the mission and if they could have reports on that. Dr. Gregurick responded that they were as engaging as the BRC and the JGI reviews. She said they are sometimes on site as was the case for an Oak Ridge SFA that she was managing. She also noted that a few members of BERAC had served on those SFA review panels so there was no loss of rigor in managing or reviewing the SFAs. She added they were a significant investment for their portfolio and they took the responsibility seriously. She said the SFAs presented their work at their upcoming Genomic Science Meeting so that would be an active way to engage and see what they were doing.

# CONTINUED DISCUSSION OF THE CHARGE: TECHNOLOGY IMPLEMENTATION FOR LONG TERM VISION

Dr. Stacey said that Dr. Remington had some information to share on the big data initiative.

Dr. Remington referred to a document that had been the product of an inter-agency working group related to big data. She advised the working group was charged out of the Networking IT Research and Development sub-group and she said she was the co-chair on the Senior Steering Group for Big Data. She noted that she could not go into great detail but wanted to bring to their attention the fact that the group had been working for nine months. She said that the group had worked hard to try and come up with a list of things that cut across agencies in terms of tackling big data. She said that Dr. Stacey had mentioned data integration and bringing data sources together and working at a particular angle and she felt that that would fall right into the bigger scheme of the initiative. She volunteered to circulate information on the vision and goals of that initiative as well as things identified as cross-agency challenges. She said there was a White House sponsored announcement of the initiative coming up and she said if they were inclined to have a workshop that could be part of the announcement as well.

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Dr. Stacey asked when the report might be released. Dr. Remington stated the working group had come up with several documents as interim deliverables to OSTP (Office of Science and Technology Policy). The initiative was planned to be announced at the end of March and there was a solicitation in the works. She stated for the DOE that Dr. Laura Biven had been the contact person.

Dr. Stacey confirmed that his plan after the meeting was to contact the Chairs of the other advisory committees and see if the idea of that kind of a workshop resonated with them. He noted he would also talk to Dr. Weatherwax and touch base with Dr. Biven.

Dr. David Thomassen said in a reminder to BERAC that they had a teleconference meeting in June of 2011 and each of the DOE, SC advisory committees was asked to put together a report and that was used as a basis for the Office of Science response to the broader initiative. He said that within the SC there was a great diversity in the openness and accessibility of data from the different programs. He said that for the most part the BER programs were at the forefront of that in terms of most of the data generated by most of the science they supported was pretty publicly assessable.

Dr. Stacey asked if BERAC were to push for a meeting that would focus specifically on computational approaches to data integration in which case the data in a way would be generic, would that be something that would resonate with that committee. Dr. Thomassen said he thought it would. He suggested that Dr. Stacey might want to talk to Dr. Biven because the Office of Advanced Scientific Computing had been running a series of workshops on that topic.

Dr. Stacey asked if any members had given additional thought about the report they had to submit.

A member said that in light of Dr. Curry's talk that they thought there was a need to put something in there about a tool or a framework about, or a community consensus as to what is needed for verification and validation of climate models. She thought that part was missing and also uncertainty quantification. She said there was a whole area of sensors and she wondered if there wasn't something needed there but she expressed the opinion that they might not be the correct group to address that.

A member said that with regard to sensors the forward-looking thing was to bring in the emerging technologies into it more. She thought that DOE and NASA would be the agencies that could really see what it might look like.

A member referred to the modeling and thought that there might be new ways of conceptualizing and approaching the modeling as well as multi-scaling across different types of domains. She said modeling was a key component of all of their BER efforts and a hallmark. She thought they could bring together the ASCR community, the mathematicians and computational scientists with them to push the envelope both on the new approaches as well as multi-scale approaches.

A member asked if they were considering moving from the molecular scale up to the global scale would they run into language problems. She was not sure of the difference, for example, of the difference between local or regional scales.

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A member said that in addition to identifying tools and the important tools that they were on the verge of having or could have, he thought it would be helpful in the report to identify a subset of big ideas, of questions that the tools could be used to address. He gave several examples and said one was soil metagenomics and linking foreign to function that would range, a function ranging from soil carbon transformations to aerosol formation in the atmosphere. He said integrated greenhouse gas dynamics might be another big area.

Dr. Stacey said he wanted to talk about the way forward and he proposed that they do the following. He said he already had some edits from several members that he had not yet incorporated into the document. He asked all members who had not edited the document, read it and use track changes to edit it or just put comments in it, to do so and send them to him as soon as possible. He said they would then move toward a new draft of the report that could be worked on from there. He said that they would reconvene the subcommittee and he had asked Dr. Curry and Dr. Gary Sayler to join the subcommittee to get some new perspectives. He said that he wanted to change the discussion of the subcommittee so that they move from a general overall forum kind of discussion into more specifics. He said he liked the idea of using specific examples or grand challenges to demonstrate how the tools would be used and demonstrate their need, and to make the report more visually appealing. He added moving forward from that they might need to have a BERAC conference call and this could be scheduled and it would be announced subject to the open meeting rules. He said alternatively they could wait for the discussion in June but he said he would see how the subcommittee was working before a decision was made. He thought that if they had a report that they felt could be discussed and voted on in June then waiting to June might be fine. However if more BERAC input was needed then a conference call might be needed.

Dr. Stacey asked if there were any further comments about the process of moving the report forward. No comments were made and so he confirmed that the process he proposed would proceed.

He asked if there were any public comments, to give a name for the record.

### **PUBLIC COMMENT**

#### Dr. Jim Hack, Oak Ridge National Laboratory

Stated that in light of the presentation on the state of climate modeling he thought it might be useful to have at the next BERAC meeting some talks on the BER program in climate modeling and the sorts of things that are being addressed by the program in the context of much broader, international efforts.

Dr. Stacey noted that a subject he had wanted to bring up was the idea of being proactive in making suggestions to the BER and the SC about issues that BERAC should be looking at and he asked if verification and validation of climate models was a topic that should be considered.

A member thought it was important but it did not have to be restricted to climate models. He thought it could spread across many things they were doing.

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Dr. Stacey said that BERAC could make a recommendation of such a workshop.

### **ADJOURNMENT**

The Biological and Environmental Research Committee adjourned for the day at 12:00 Noon.