

**Minutes of the
Biological and Environmental Research Advisory Committee Meeting
February 23–24, 2010
Hilton Hotel, Gaithersburg, Md.**

BERAC members present:

Gary Stacey, Chair	Gregory Petsko
Janet Braam	David A. Randall
Robert E. Dickinson	Karin Remington
James R. Ehleringer	G. Philip Robertson *
Joanna S. Fowler	Gary Sayler
Paul Gilna *	James M. Tiedje (Tuesday only)
Susan Hubbard *	Judy Wall
Andrzej Joachimiak	Warren M. Washington
L. Ruby Leung *	Raymond E. Wildung
Gerald Mace *	Mavrik Zavarin
Joyce E. Penner	Minghua Zhang *

BERAC members absent:

Stephen R. Padgett	Herman Shugart *
Margaret A. Riley	

Before the meeting, the new members of the Committee (*) were sworn in by members of the Department of Energy (DOE) Human Resources Department.

The Chairman, **Gary Stacey**, called the meeting to order at 9:00 a.m. He asked each Committee member to introduce himself or herself.

Patricia Dehmer, Deputy Director for Science Programs, gave a presentation on the Office of Science (SC) rollout package used to brief Congress on the FY11 budget request.

The SC FY11 budget request to Congress shows the priorities of the Office of Science, Assistant Secretary, Secretary, and Office of Management and Budget. Basic Energy Sciences (BES) goes up 12%; Advanced Scientific Computing Research (ASCR), 8%; and Biological and Environmental Research (BER) 4%. There are more modest increases for the other offices. The overall SC increase is 4% (actually 6.1% after earmarks are deducted).

SC supports 27,000 Ph.D.s, graduate students, undergraduates, engineers, and technicians and 26,000 users of open-access facilities. It provides support to 300 leading academic institutions and all 17 DOE laboratories. The FY11 budget advances discovery science and invests in science for national needs in energy, climate, and the environment; national scientific user facilities; and education and workforce development.

There is money for the design of new internal combustion engines in the ASCR budget. The BER budget emphasizes climate modeling. Fusion has a decrease because of the International Thermonuclear Experimental Reactor (ITER). High Energy Physics has

mostly the continuation of existing programs. Nuclear Physics has \$300 million for the upgrade of the Thomas Jefferson National Accelerator Laboratory. Continued support for fundamental research is expected to be strong in the coming years.

In discovery science, funding is included for an Energy Innovation Hub for Batteries and Energy Storage and enhanced activities in climate science and modeling. The Energy Frontier Research Centers (EFRCs) account for a \$66.2 million increase in BES. The Leadership Computing Facilities operations and preparation for next generation of computer acquisitions for science and technology modeling and simulation received \$34.8 million in ASCR. Multiscale modeling of combustion and advanced engine systems accounts for an increase of \$20 million in BES.

In scientific user facilities, facility construction is fully funded, and projects are meeting baselines; 28 scientific user facilities will serve more than 26,000 users; and several new projects and Major Items of Equipment are initiated.

In education and workforce development, there are expansions of the SC Graduate Fellowship Program and the SC Early Career Research Program (ECRP). The first wave of awards in the ECRP has been made. The SC ECRP started with \$100 million of American Recovery and Reinvestment Act (ARRA) funding; there are now 60 new early career scientists being funded. The SC offices and programs themselves will fund this program in the future, and the number of researchers will increase to about 170. The Secretary is incredibly supportive of the ECR and Graduate Fellowship programs.

In FY10, three hubs were funded, with SC leading the Fuels from Sunlight Hub. The hubs received \$25 million each, with an additional \$10 million of startup money the first year. In FY11, the Energy Innovation Hub for Batteries and Energy Storage will be added to SC's portfolio. The Secretary is very passionate about these hubs.

BER increases funding by more than \$21 million for climate modeling and climate research, a high priority of the Secretary.

A 2-petaflop machine (the Jaguar) is operating at Oak Ridge National Laboratory (ORNL). It is the fastest nonmilitary computer in the world. An exascale computer (1,000 to 10,000 times faster than the Jaguar) is being considered by DOE. The Department is interested in pushing high-performance computing.

A lot of work has been done on the simulation of internal combustion engines, and that work will continue.

The synchrotron radiation light sources have had a massive impact on structural biology. The number of users of the light sources has grown rapidly; one-third of the users are structural biologists.

\$75 million will support the fourth year of operations of the three Bioenergy Research Centers (BRCs). Each BRC has a lead institution but also a *lot* of partners.

Advances in DNA sequencing and analysis have revolutionized the study of biology through rapid genome mapping at the Joint Genome Institute (JGI) and like facilities. There are increases in the budget to support this genomic revolution.

QUESTIONS/COMMENTS

Stacey noted that the Science and Technology Committee is considering the FY11 budget now and that the chair is supportive of re-authorizing SC programs. Dehmer responded, yes, they are supportive. In the out years, the President will hold discretionary funding flat but has committed to the doubling of research funding. The National Institute

of Standards and Technology (NIST) is way up; SC is up 6%. The nation is facing an election year and economic realities.

Dickinson asked if any research was being conducted on methane hydrates as a greenhouse gas or as a fuel. Dehmer replied, yes and that topic was moved from the Office of Fossil Energy to SC (BES) for that reason.

Petsko noted that infrastructure funding actually went down in the FY11 budget request. Dehmer pointed out that some construction projects have been completed and a few new ones have been started. New projects will continue to be started each year.

Petsko asked if there was any Department of Defense (DoD) cooperation on batteries and energy storage. Dehmer answered that there was cooperation with DoD and with other agencies on those topics; SC's work will be on fundamental science.

Wildung noted that the Advanced Research Projects Agency-Energy (ARPA-E) has \$500 million and asked what the general relationship was between SC and ARPA-E. Dehmer responded that the Director of ARPA-E is very interactive with the leadership of SC and with the associate directors in each office. He has set up a panel of advisors drawn from that leadership.

Gilna asked where DOE saw itself in interagency climate research. Palmisano said that she would cover that subject in her presentation.

Anna Palmisano, Associate Director for Biological and Environmental Research, was introduced to give an overview of the activities of BER. She recognized by name the members who had rotated off the Committee and she welcomed the new members.

She acknowledged BER-funded scientists winning prestigious awards since the last BERAC meeting. She congratulated Joanna Fowler (BERAC member) and Craig Venter for receiving the 2009 Presidential Medal of Science. The 2009 Nobel Prize in Chemistry went to Venki Ramakrishnan, Thomas Seitz, and Ada Yonath; Ramakrishnan started his work at Brookhaven National Laboratory (BNL) with BER funding. Sallie Chisholm won the Alexander Agassiz Medal and Watt Webb won the Alexander Hollaender Award. A Presidential Early Career Award for Scientists and Engineers (PECASE) went to Alexandre Tartakovsky of Pacific Northwest National Laboratory.

BER provides the foundational science to (1) support the development of biofuels as major, secure, and sustainable national energy resources; (2) understand the potential effects of greenhouse-gas emissions on Earth's climate and biosphere and the implications of these emissions for our energy future; (3) predict the fate and transport of contaminants (particularly radionuclides) in the subsurface environment at DOE sites; and (4) develop new tools to explore the interface of biological and physical sciences. The driving science questions are

- What are the roles of the Earth systems (atmosphere, land, oceans, sea ice) in determining climate?
- How is information stored in a genome translated into active microbes, plants, and ecosystems and their functions?
- And what are the biological and physical forces that govern the behavior of Earth's subsurface environment?

The BER FY11 Congressional budget request breaks down into \$237 million for Biological Systems Science Research, \$204 million for Climate and Environmental Sciences Research, \$101 million for Climate and Environmental Facilities and

Infrastructure, and \$85 million for Biological Systems Facilities and Infrastructure (rounded).

In the Biological Systems Science Division (BSSD), Genomic Science has increased; Radiological Sciences has stayed about the same; Ethical, Legal, and Societal Issues has stayed about the same; Medical Applications has decreased slightly; Biological Systems Facilities and Infrastructure has stayed about the same; and the Small Business Innovative Research/Small Business Technology Transfer (SBIR/STTR) Program has increased slightly.

Genomic Science requested \$177 million for foundational genomics research (\$40 million), genomics analysis and validation (\$10 million), metabolic synthesis and conversion (\$39 million), computational biosciences (\$13 million), and the BRCs (\$75 million).

The BRCs are completing their third year of funding in FY10. They are the Great Lakes Bioenergy Research Center (GLBRC), the Joint BioEnergy Institute (JBEI), and the BioEnergy Science Center (BESC). BER conducts annual scientific and management peer reviews for each of these, and the reviews have been very positive. BER manages against milestones for scientific progress, and the centers have been on or ahead of schedule.

In Radiological Sciences, radiochemistry and imaging instrumentation with \$18.4 million is developing synthetic radiochemistry, radiotracers, and multimodal tracers; advanced imaging instrumentation for new opportunities to study microbial and plant metabolism and for tracking dynamic biological processes in the environment. A community workshop was held in November 2008. With \$24 million for radiobiology, BER is supporting research that underpins radiation protection standards and focusing on models integrating responses in tissue and organisms with epidemiology.

With \$5 million, BER's Ethical, Legal, and Societal Issues Program will continue to focus on systems microbiology, synthetic genomics, sustainability for bioenergy, and nanotechnology in the environment.

With \$4 million, the Medical Applications Program is transitioning artificial retina research to a development and application stage. The National Institutes of Health (NIH) continues to fund animal testing studies and clinical trials.

With \$15.7 million, Structural Biology Infrastructure will continue to support access for the biology community to structural biology beamlines and instrumentation at DOE national user facilities, coordinate management and maintenance [with NIH and the National Science Foundation (NSF)] of 22 experimental stations at DOE synchrotron and neutron sources, and continue to expand the user community to include subsurface scientists.

The Joint Genome Institute (JGI) with \$69.3 million is improving its annotation tools and addressing grand challenges.

In Climate and Environmental Sciences, there are significant funding increases (\$19 million increase overall). With \$28.4 million (\$1.9 million increase), Atmospheric System Research seeks to determine the relationships between clouds and atmospheric radiative-transfer processes (i.e., aerosol properties, effects, and transformations on Earth's energy balance, aerosol-cloud-precipitation interactions, polar clouds and aerosol interactions, and cloud properties and effects on Earth's energy budget) and then to

incorporate results into climate models. There is a new Atmospheric System Research community-based science plan.

With \$81.5 million, Environmental System Science is trying to determine the impacts and feedbacks of climate change on terrestrial ecosystems with a focus on the arctic tundra and to estimate cycling and storage of carbon in terrestrial ecosystems as part of the AmeriFlux network. Some other projects will decline.

With \$49.9 million, Subsurface Biogeochemical Research will support an interdisciplinary approach that includes microbiology, geochemistry, and hydrology; focus on the mobility of metals and radionuclides in the subsurface; and will continue to couple lab-based research with Integrated Field Research Centers. An August 2009 community workshop defined the future research needs and approach.

With \$85.6 million (\$15.8 million increase), Climate and Earth System Modeling will improve the fidelity of climate predictions at higher resolution; develop diagnostic tools to evaluate global and regional models; continue development of a comprehensive coupled Earth system model at high resolution; improve the representation of physical, chemical, and biogeochemical processes in models; provide scientific insights to the complex interactions of human and natural systems; and explore implications of science and technology decisions and innovations on our energy, environmental, and economic future.

The Atmospheric Radiation Measurement Climate Research Facility (ACRF) includes two mobile and three fixed sites. It will receive increased support for new instruments and their deployment.

The Environmental Molecular Sciences Laboratory (EMSL) has added several new instruments to study biological interactions and dynamics, geochemistry/biogeochemistry and subsurface science, the science of interfacial phenomena, and aerosols.

The BER priorities for FY11 lie in genomic science and climate science. In genomic science, they are to develop new genomic and analytical technologies for dynamic measurements of biological systems and to develop a new data-integration and modeling framework for systems biology. In climate science, they are to develop the next-generation 3D cloud parameterizations; to improve representation of aerosol indirect feedbacks and uncertainty quantification in models; to support dataset conversion, model-development testbeds, and the transition of climate models to new computing architectures; and to continue to support operations for new ARRA instruments at the ACRF to improve cloud and aerosol representation in climate models.

ARRA investments were made in the ACRF to enhance the current measurement base to provide new knowledge and improve the predictive performance of climate models. \$60 million were invested for instrumentation and research infrastructure for the fixed and mobile ACRF facilities. At EMSL, \$60 million were invested in 25+ leading-edge experimental capabilities, including nuclear magnetic resonance (NMR) spectrometers, mass spectrometers, molecular/microscopy imaging capabilities, and nano- and molecular-level characterization instruments. More than 175 purchases are expected. At the BRCs, \$13.5 million were invested for infrastructure for plant feedstock genome analysis and characterization (purchase of dozens of new instruments). At the JGI, \$13.1 million were invested in infrastructure for genome sequencing, analysis, and characterization for plant feedstocks; information technology (IT) servers; compute nodes; networked data storage; sequencing reagents; and a next-generation sequencer.

\$4.9 million were invested for the Integrated Assessment (IA) Research Program in computing, archive storage, and visualization equipment for integrated-assessment modeling. For Knowledgebase (Kbase) R&D, \$3.2 million were invested in conceptual design and planning for a Systems Biology Knowledgebase, for which three of five workshops have been held and five software projects have been initiated.

The early career awards are supporting the next generation of young scientists. This is the largest effort of its kind in DOE history aimed at the next generation of scientists. David Thomassen is the overall lead for BER, with Marv Stodolsky for BSSD and Bob Vallario for the Climate and Environmental Sciences Division (CESD). The early career is defined as no more than 10 years past Ph.D., and the initial funding is from the ARRA but involves a long-term commitment from BER. There were 271 proposals to BER. It held 10 review panels with 147 reviewers with 3 or more reviews per proposal; about 25 BER staff were involved. Eight awards (three laboratory and five university) were made with a 3% success rate. The most meritorious proposals from each division (BSSD and CESD) were recommended to the Associate Director for funding.

The BER 2010 SC Early Career Award recipients were William Gustafson, Pacific Northwest National Laboratory; Matias Kirst, University of Florida; Uljana Mayer, Pacific Northwest National Laboratory; Nathan McDowell, Los Alamos National Laboratory; Victoria Orphan, California Institute of Technology; Jonathan Schilling, University of Minnesota; Timothy VanReken, Washington State University; and Mort Webster, Massachusetts Institute of Technology.

BSSD coordinates with ASCR through Scientific Discovery through Advanced Computing (SciDAC) for bioenergy and in computational biology and bioinformatics; with BES on beamlines for structural biology and bioenergy research; and with the Office of Energy Efficiency and Renewable Energy (EERE) (particularly its Office of Biomass Programs) for which BER provides fundamental science on new bioenergy crops, biomass deconstruction, and consolidated bioprocessing and for which ARRA-funded EERE pilot plants are located near BRCs. With the EERE Biomass Program, \$20 million of ARRA funding was received to build an integrated process development unit at Lawrence Berkeley National Laboratory (LBNL) for pilot-scale pretreatment of biomass, production of enzymes for biomass deconstruction, and fermentation capacity for advanced biofuels production; for dedicated access to all BRCs, and for general access (academic and industrial).

BSSD also coordinates with the U.S. Department of Agriculture (USDA) on feedstock genomics research; with NIH on radiochemistry, structural biology user stations, and planning a joint workshop on the integration of physical science with biological science with the National Institute of General Medical Sciences; with NSF on a protein databank (together with NIH); and with the National Aeronautics and Space Administration (NASA) on low-dose radiation biology.

CESD coordinates with ASCR through SciDAC for climate modeling and for subsurface modeling; with BES on beamlines for biogeochemistry and geosciences; with Environmental Management (EM) on the science underpinning contaminant fate and transport; and with Legacy Management on the science underpinning tools for long-term contaminant fate, transport, and monitoring.

CESD also coordinates with the 13 agencies involved in the U.S. Global Change Research Program, which meets every three weeks and is overseen by the Office of

Science and Technology Policy (OSTP). Four agencies have the most climate-science funding: NASA, NOAA, NSF, and DOE. It also coordinates with the Strategic Environmental Research and Development Program (SERDP) of DoD and will have a new solicitation with NSF and USDA on regional climate modeling in March 2010.

Committee of Visitors (COV) reviews assesses the processes used to solicit, review, recommend, and monitor; proposals for research in SC programs; the breadth, depth, and national/international standing of portfolios; and the management and oversight of DOE national user facilities. They are conducted every 3 years and review all program and facility-management activities during the past 3 years. Reviewers are provided access to all program-related and facility documentation, including previous COV findings. Findings are presented to the relevant federal advisory committee, and reports are submitted to the SC Director.

A COV Review of CESD will be held July 21-22, 2010, at DOE headquarters in Germantown, Md. It will be chaired by Judy Wall (BERAC). The COV staffing and review logistics are in progress. It will review CESD programmatic actions for FY07–FY09.

In personnel, BER is actively recruiting a Director of CESD; had to re-post the recruitment for a replacement for Roger Dahlman; is recruiting a replacement for Anjali Bamzai, who moved to the NSF; was joined by Shireen Yousef as Science Assistant in BSSD, and joined by Eileen Knox as secretary for CESD.

BER outreach and communications need to tell the success stories. The BER team, led by David Thomassen together with Betty Mansfield's group at ORNL, has come up with BER and division "4-pagers," program-element "2-pagers," a BER poster, key workshop summaries, and BER presence at key scientific meetings.

BERAC has been charged to identify grand-challenge science, answering the questions

- What are the greatest scientific challenges in biology, climate, and the environment that DOE will be facing in the long term?
- How should BER be positioned to address those challenges?
- What fields of science are needed to achieve future mission challenges?
- What new and innovative tools are needed to advance BER science?
- How can the workforce of the future be trained in integrative system science?

A BERAC Grand Challenge Workshop is being held March 3-4, 2010, to address these questions. BER is following the "Basic Research Needs" model developed by Pat Dehmer in BES. This activity will be described in greater depth later in the meeting.

QUESTIONS/COMMENTS

Stacey noted that DOE/BER may be one of the "big four" of the U.S. Global Change Research Program (USGCRP), but its \$20 million for climate research seems small. Palmisano replied that DOE also provides the ACRF and computing facilities to others. BER's role is in strategic areas. A lot of the funding of other agencies is in satellites, which are very expensive.

Washington asked about overlap with the NSF's National Ecological Observatory Network (NEON). Palmisano answered that there was good coordination with NEON and that the effort will expand into the Arctic.

Wildung stated that the BER programs responded wonderfully to the ARRA funding opportunity. Palmisano said that Dehmer should receive full credit for that response.

Ehleringer noted that NEON offers many opportunities for investigating climate change and fates, but it seems to be backing away from climate-change experiments. Palmisano said that the Office will follow up on that.

Zhang asked about coordination with ASCR. Palmisano replied that ASCR has SciDAC and INCITE [Innovative and Novel Computational Impact on Theory and Experiment] to provide computational resources that BER-funded scientists use.

Gilna asked if there were any links with ARPA-e. Palmisano said that she serves on one of ARPA-E's advisory panels. The Director of ARPA-e understands that BER will be important in the success of his program.

Braam asked what has actually come out of the BRCs. Palmisano stated that Sharlene Weatherwax will cover that information in detail.

A break was declared at 10:38 a.m. Meeting called back into session at 11:00 a.m.

Jeffrey Marqusee (Executive Director, Strategic Environmental Research and Development Program (SERDP)) provided an overview of DoD's environmental technology programs, the Strategic Environmental Research and Development Program (SERDP, a science and technology program funded at \$68 million) and the Environmental Security Technology Certification Program (ESTCP, a demonstration and validation program funded at \$70 million). These programs assess requirements of the military services, conduct basic and applied research, perform advanced development, conduct demonstration and validation, and accomplish implementation.

The environmental drivers include groundwater, soils, and sediments; a large unexploded ordnance liability; and emerging contaminants. DoD is an enormous industrial infrastructure with enormous environmental issues. The agency is committed to reaching the sustainability of its ranges, facilities, and operations by dealing with such issues as maritime threatened and endangered species, toxic air emissions and dust, noise, urban growth, and climate change.

SERDP was established by Congress in FY91 as a tri-agency program with a DoD, DOE, and Environmental Protection Agency (EPA) partnership. SERDP is a requirements-driven program that identifies high-priority environmental science and technology investment opportunities that address DoD requirements. It conducts advanced-technology development to address near-term needs and fundamental research to impact real-world environmental management.

Its director reports to the SERDP Council and has a Scientific Advisory Board, an Executive Working Group, and a Senior Technical Committee. Its extended virtual staff is multi-agency with more than 40 technical members who take on a significant time commitment.

ESTCP is a demonstration program created to capitalize on past investments and to transition technology out of the laboratory. It promotes implementation by direct technology insertion and by gaining regulatory and end-user acceptance. It has been hugely successful at this.

These programs have four focus areas: weapon systems and platforms, munition management, environmental restoration, and sustainable infrastructure. Both programs are completely competitive with minimal infrastructure.

SERDP's investments continuously evolve. Annual solicitations are structured around statements of need (SON) that reflect longer-term strategic plans to address critical needs and standalone investments addressing narrower needs. The mechanisms used to solve these problems are SERDP technical committees, workshops, special studies, the Science Advisory Board, and working groups.

SERDP does a lot of work on contaminated sediments. It has been investing in new technologies since the 1990s. It researches the impacts of in-place remedial strategies, the distribution and placement of amendments, the assessment and measurement of processes impacting the fate and transport of contaminants, ecosystem risk and recovery, and bioavailability. The DoD is a huge landholder and is concerned about the effects of climate change on those lands. It also has to address environmental restoration, requiring the development of tools to determine the environmental impacts of munitions compounds in the marine environment; groundwater fate, transport, and treatment; improved understanding of impacts to groundwater quality; assessment of source terms; and remediation of contaminated aquatic sediments. It also is concerned about the sustainability of infrastructure (e.g., climate change and Alaskan ecological systems, the behavioral ecology of cetaceans, ecological forestry and carbon management, and ecology and management of source-sink populations).

ESTCP uses broad competitive solicitations to create partnerships and conduct tests at DoD facilities. It then validates operational cost and performance and identifies DoD market opportunities. ESTCP 2011 topics include protection and remediation of contaminated groundwater; military munitions detection, discrimination, and remediation; ecosystem service methodologies and tools for DoD installations; and energy efficiency and renewable energy for DoD installations. It funds individual investigators to develop tools that can be used by managers to address problems at their sites.

There has been a sharp change at DoD in the past year. In the past two weeks, the *Quadrennial Defense Review Report* has come out. It calls for crafting a strategic approach to climate and energy. SERDP and ESTCP are funding climate-change R&D to understand impacts, vulnerabilities, and adaptation and mitigation strategies. Sea-level rise is a threat to coastal military installations. Energy use is a huge concern because DoD has direct costs for fuel of \$20 billion per year and \$4 billion in energy costs at facilities. The 40% of energy use occurring in infrastructure is the most likely place to deploy efficiencies.

DoD has 545,700 facilities, 316,200 buildings, and about 2.2 billion sq ft, most of which is not new. These facilities will be used as testbeds for energy conservation. DoD is working with DOE/EERE to reduce energy costs, lower DoD's carbon footprint, and improve security. A workshop will be held on environmental technology from Nov. 30 to Dec. 2, 2010, at the Marriott Wardman Park Hotel in Washington, D.C.

QUESTIONS/COMMENTS

Tiedje noted that, as BER plans for the future, there could be interaction with SERDP in multiple areas of terrestrial-landscape management. Marqusee agreed that they could

cooperate in moving up from the plot scale to the scale of manager's responsibilities. The calls for proposals do not specify particular sites but just require certain information to be pursued.

Zavarin asked how post-closure contaminant management was carried out. Marqusee responded that, in groundwater, one expected a return to drinking-water quality. That is impossible. Most places will have a 30-year horizon (with more management required after that).

Wall said that the amount cited seems like a modest investment for the largest industrial complex in the world. Marqusee answered that the work is leveraged with the services of logistics and maintenance programs.

Sayler noted that the Navy has an interest in biofuels and asked if there were a responsibility there. Marqusee replied, yes, as does the Air Force. The DoD can play a crucial role as an early adopter. It buys fuel as a commodity. The lead should therefore come from DOE. Investments are being made now in understanding the environmental impacts of turbine engines.

Philip Robertson (BERAC) was introduced to talk about bioenergy and sustainability.

The legislated Biofuel Goals were set by the U.S. Energy Independence and Security Act of 2007 (EISA) to be 22% of the transportation fuel mix in 2022 from 36 billion gallons (bgal) of ethanol (15 bgal of grain-based ethanol and 21 bgal of advanced ethanol). The current U.S. ethanol production is 14.6 billion gallons per year (bgal/y) from grain. Cellulosic ethanol production today is essentially zero but is ramping up.

Cellulosic feedstocks need pretreatment to open the structure to enzyme attack. It is hoped that enzymes will act on any cellulosic materials, but there are no guarantees.

The goal is to displace 142 billion gallons of gasoline per year. To do that, 107 bgal/y of biofuels will be needed in 2050, which would require 42 billion bushels of grain or 902 million metric tons (MMT) of cellulosic biomass. Current annual cellulosic feedstock productions are 109 MMT of forest products, 90 MMT of municipal solid waste, and 55 MMT of corn stover. Some of these sources have serious sustainability questions. To meet the needs of 2050, an additional 650 MMT of biomass would be required. The land area needed would be 86×10^6 ha.

The hope is to boost productivity by improving land management and genomics. The energy required to pump groundwater to irrigate this amount of land quickly outstrips the energy gained by these biofuels. These systems have to be profitable, be carbon negative, be nutrient and water conservative, have biodiversity benefits, provide food and energy security, and promote rural community health.

A social-systems framework has been developed that links social and geophysical aspects through pulses (fire, drought, etc.), pressures (climate change, sea-level rise, etc.), and the production of ecosystem services (water cleansing, runoff retention, food production, etc.). Perceptions about human outcomes can lead to changes in how the ecosystem services are delivered and will influence human behavior (farmer decisions and actions, consumer preferences, regulations, technology development, market performances, etc.).

These considerations have led to a sustainability research roadmap. It is now known that grain-based fuel comes with environmental costs that are not different from those for

conventional food crops. They will not have much effect on climate stabilization. There will be a greater intensification of existing farmscapes with associated erosion, nitrate and phosphorus loss, pesticide loading, and biodiversity loss. Best-performance practices can mitigate many of these effects.

Cellulosic crops could provide a major contrast by using perennial herbaceous and woody crops while providing landscape diversity, no carbon debt, and ecosystem services. Life-cycle analysis of carbon impacts must consider agronomic CO₂ costs, biorefinery CO₂ costs, and land-use-conversion costs. The revised Renewable Fuel Standard (RFS2) greenhouse-gas thresholds have been specified in EISA. The indirect land-use effects (e.g., displaced food production) have certain effects.

Agriculture can play a role in stabilizing CO₂ by reducing fossil-fuel consumption, identifying CO₂ sinks and sequestration rates, and reducing non-CO₂ greenhouse gases. The atmospheric carbon content is currently increasing by 4.1 PgC/y. The hope is to reduce this value to zero. Currently, the best way to sequester carbon is to take it out of the atmosphere with plants and to “bury” that carbon. Sequestration has the potential for removing 0.3 to 0.5 PgC/y by increasing carbon inputs with crop residues and cover crops and/or by slowing decomposition via no-till agriculture.

The Kellogg Biological Station’s Long-Term Ecological Research site continues to investigate annual grain crops with conventional tillage, no-till, low-input with legume cover, and organic with legume cover along with perennial biomass crops and unmanaged communities. Annual grain crop carbon accumulation rates are: with conventional tillage (0 g/m²-y), no-till (30 g/m²-y), and organic with legume cover (8 g/m²-y). The accumulation rates for perennial biomass crops are 44 g/m²-y and 32 g/m²-y for alfalfa and poplar, respectively. Unmanaged successional communities accumulated carbon at the rates of 60 g/m²-y during early succession, <11 g/m²-y during mid-succession, and 0 g/m²-y during late succession.

Other radiatively active gases must be considered, especially methane and nitrous oxide because their global warming potentials are much greater than that of carbon dioxide and because agriculture produces 55% of the anthropogenic methane and 80% of the anthropogenic nitrous oxide globally. Not all biomass crops are equal in this regard; poplars and successional forests produce very little nitrous oxide. Fertilizer applications can exceed the amount of nitrogen that plants can absorb, releasing nitrous oxide to the atmosphere. For methane, increasing the sinks can draw down methane emissions to the atmosphere; reducing the sinks significantly increases the methane release. Mature forests consume far more methane than does agriculture.

Nitrous oxide is the largest source of global warming potential, but this gas is not well quantified today. Compared to grain crops, alfalfa has a lower farming cost and a greater soil-carbon gain. Early succession forest has very little farming cost, produces a large nitrous oxide drop, causes a large soil-carbon gain, produces less biomass than alfalfa, but has the same net benefit as alfalfa. Thus, among crops studied, alfalfa and early successional produce the greatest net mitigation benefit, and fertilized successional yields are similar to on-farm switchgrass yields.

In conclusion, land requirements are substantial; outcomes that provide multiple benefits are possible; and the best biogeochemical outcomes will depend on the choice of crops, management practices, and location. What is needed is a comprehensive science

understanding at the systems level along with a willingness to incentivize environmental performance.

QUESTIONS/COMMENTS

Leung asked how important the water requirement was. Robertson replied that it is crucial, particularly the water needed for irrigation. If one replaces current vegetation with lower-efficiency vegetation, one runs into trouble. Inversely, one can reduce the runoff to streams. That is good for nitrate contamination, but bad for water quantity. Evapotranspiration in corn occurs only during a few months of the year; but from perennial crops, it occurs all year long.

Wall asked how many refineries would be needed. Robertson answered that 60 km would be the maximum transport, and therefore there would be pretreatment centers in each county.

Ehleringer asked what the impact would be if our society did not eat beef. Robertson replied that there would be a reduction in corn use of a factor of 10 or so.

A lunch break was declared at 12:44 p.m. The meeting was reconvened at 2:01 p.m.

Michael Kuperberg was introduced to provide an overview of BER's Climate and Environmental Sciences Division (CESD).

A number of solicitations are open at this time: university solicitations are on (1) research in integrated assessment inter-model development, testing, and diagnostics and (2) modes of low-frequency variability in a changing climate. Those for national laboratories are on (1) climate uncertainties at regional and global scales and (2) earth system modeling: advanced scientific visualization of ultra-large climate data sets.

Upcoming solicitations include one on terrestrial ecosystem science that should be out in one week, one for subsurface biogeochemical research that is in development for FY11 funding, one on atmospheric system research that is in final development, and an NSF-USDA-DOE solicitation on decadal and regional climate prediction using Earth system models.

Science highlights from the Division include

- The first study to indicate that the status of the Bering Strait may have played an essential role on past climate changes (meridional overturn and ice-sheet development).
- Early results from a successful simulation of the magnitude of the abrupt Bolling-Allerod warming is the first coupled global climate model simulation of the transient climate evolution since the Last Glacial Maximum.
- A new process has been developed for creating plausible scenarios for climate change research and assessment and including four standardized scenarios.
- ARM in January conducted a new aircraft campaign to obtain a new and comprehensive set of in-cloud measurements about the size and number of ice crystals that make up cirrus clouds
- The ARM Mobile Facility (AMF) is continuing its deployment in the Azores to study marine clouds.
- ARM ARRA activities are on track and new instruments are expected to be operational in September.

- Experiments for 2011 include a joint effort with NASA on precipitation, Madden Julian Oscillation experiment in Manus, AMF2 in Colorado, and AMF1 in Ganges Valley.
- A team of ARM researchers presented a framework for interpreting the chemical transformations and physical characteristics common to organic aerosols from diverse human and natural sources, which holds promise for enabling scientists to build model descriptions of the behavior of aerosol formation.
- At EMSL, analyses using a battery of analytical techniques and the Advanced Photon Source (APS) enabled identification of oxidized and reduced uranium on the pyrite surface.
- Subsurface biogeochemical research demonstrates a biochemical mechanism for the microbial respiration of extracellular solid phases such as metal oxides, which is important for understanding bacterially mediated metal and radionuclide reduction in subsurface environments.

In terrestrial ecosystem research, plans are proceeding for the next-generation ecosystem experiment (arctic tundra warming) with infrastructure prototype development under way.

A large-scale northern Minnesota bog warming/elevated-CO₂ experiment is underway. It is a joint effort between ORNL and U.S. Forest Service.

The Division is also supporting a range of in situ warming and precipitation manipulation experiments. How plant community species composition is being affected by climate change treatments and mechanisms of drought-induced plant mortality are being elucidated. Effects of warming on insect populations are being quantified at the genetic level.

Future CESD activities include principal-investigator meetings for the Atmospheric System Research (ASR) Program (March 15-19 at the Marriott Bethesda North Hotel in Bethesda, Md.), for Subsurface Biogeochemical Research (March 29-31 at the JW Marriott, Washington, D.C.), and the Climate Change Modeling Programs – Integrated Assessment Science Team (March 29-April 2 at the Gaithersburg Hilton) and the Climate Roadmapping Workshop.

QUESTIONS/COMMENTS

Gilna stated that there is a huge opportunity for connections between these two disciplines. Kuperberg replied, yes, there are. They are in the free-air carbon enrichment (FACE) experiments and the genomics laboratory; the next-generation experiment will use the instruments and personnel of the whole community. There will be a workshop on genomic cycling. An effort is being made to tie subsurface science in with carbon cycling.

Mace asked if the modest increase in the budget was a concern. Kuperberg answered affirmatively. An investment in personnel is needed to get a good payoff in the instrumentation investment.

Mace noted that ARM has been flat-funded for 15 years and has lost funding in real dollars. Kuperberg said that they were pleased with the increase that was received. Palmisano said that the increase that was received will be used to get full advantage of the recent investments in instrumentation.

Zhang asked how the ASCR funding was being used. Kuperberg said that ASCR's investment is in the technology. This effort is based on the climate data to be visualized.

Gilna asked if the ARM program still has access to unmanned aerial vehicles (UAVs). Kuperberg replied that ARM does not have ownership of any UAVs. It uses other agencies' capabilities.

Wildung asked if there were any efficiencies that have been gained through the reorganization processes. Kuperberg replied that, since the consolidation, the climate program has changed to incorporate and coordinate a variety of disciplines. There is an interest in bringing together the subsurface and carbon-cycle programs.

Sharlene Weatherwax was asked to review the activities of the Biological Systems Science Division.

Current solicitations include

- Biological Systems Research on the Role of Microbial Communities in Carbon Cycling, an outgrowth of the workshop report
- Computational Biology and Bioinformatic Methods to Enable a Systems Biology Knowledgebase, the plan for handling all the data in the future
- Joint USDA–DOE Plant Feedstock Genomics for Bioenergy (proposals have just come in)
- Radiochemistry and Radionuclide Imaging Instrumentation Research (recently released)

Upcoming solicitations include one in the planning stages of the Genomic Science Research Program to link genomics with imaging technologies. The call will be out in April.

A workshop on opportunities in biology at the extreme scale of computing was held August 17-19, 2009, in Chicago. Its goal was to examine the role of extreme-scale computing in biological research and the overlap to further DOE missions in bioenergy, bioremediation, and the global carbon cycle. The workshop was divided into five focus areas: tissues, organs, and physiology modeling; pathways, organelles, and cells; macromolecular proteins and protein complexes; populations, communities, ecosystems, and evolutionary dynamics; and the data analysis, imaging, and visualization required. It found that computing at this scale will drive new hardware architectures to enable multi-scale biological computations that require significant advances to change the development of algorithmic, analytical, mathematical and statistical methods in order to meet these computational and data-rich challenges. Also, advances in data, image, and visual analyses are as essential as new methodologies in the extreme-scale to enable biological-science-driven discovery processes.

Research highlights include:

- Determining the structures of the four shell proteins and showing how changes in one protein impact overall microcompartment shell shape
- Sequencing a 1.1 Gb soybean genome with assembly and integration with physical and high-density genetic maps, identifying 46,000 putative genes
- Multiplex automated genome engineering to concurrently engineer multiple target genes in a microbial biosynthetic pathway for enhanced production by using multiple cycles of oligomer-directed mismatch against target genes to generate 4.3 billion genomic variants per day

- Detecting low-dose radiation-induced bystander effects in vivo with an adoptive transfer method, which did not see a big bystander effect
- Using high-resolution secondary ion mass spectrometry (NanoSIMS) to quantify uptake and image localization of radiolabeled substrates in cyanobacteria
- Advancing research and training in radiochemistry to train the next generation of scientists in novel and innovative state-of-the-art radiochemistry research in partnership with NIH
- Inventorying maize cell-wall genes with a high-throughput screen to identify cell-wall mutants

The BRCs have finished their second year. An external review team evaluated the science and management and progress against stated milestones. The reviewers were enthusiastic about each BRC's successful transition from start up to full operational mode. All centers have demonstrated significant research accomplishments. Reviewers all expressed confidence in leadership and management by each BRC director.

Research results from the BRCs include

- Characterization of bacterial communities for growing biomass crops on marginal lands
- Mining compost for enzymes to develop novel enzymes for switchgrass degradation
- Use of a thermophilic bacterium to reduce the cost of pretreatment requirements

The Joint Genome Institute (JGI) is having an operations review March 10-11 to assess project tracking, communication with JGI users, resource optimization for operational efficiency, adoption of new technologies, and contingency planning. Its Community Sequencing Program 2011 announcement is anticipated in March 2010. It is open to large-scale resequencing of organisms, large-scale metagenome sequencing, single-cell genomes, and large-scale microbial isolate sequencing. The JGI's strategic planning is being updated with the results from the workshop on Applications of High-Performance Computing (HPC) in Genomics, which was held in January 2010.

BSSD has had or will be having PI meetings for JGI, Low Dose Radiation Research, and the Artificial Retina Program. Workshops will be held on Systems Biology Knowledgebase Conceptual Design, Critical Assessment of Functional Annotation Experiment (CAFAE), and Central DOE Institutional Review Board, and ESN [Energy Sciences Network] requirements.

QUESTIONS/COMMENTS

Tiedje stated that one should not forget the importance of reference genes in analyzing metagenomes. Weatherwax agreed. Tiedje asked about genes of unknown function. Weatherwax answered that annotation will be the key. A multipronged approach is being used:

- work at the JGI to refine methods,
- cooperation with the NIH, and
- a workshop to identify critical targets.

Joachimiak noted that only a few organisms can be cultured, so some reference genomes should be pursued. There are thousands of cellulases. He asked if there were any coordinated efforts to sort through them. Weatherwax replied that several approaches

were being taken because the cellulose is bound to many other things. An effort is being made to improve on ways to solubilize cellulose.

Stacey asked if there were any plans to sequence some basal plants to understand metabolic pathways. Weatherwax responded that the need to compare the genomes of interest was recognized. The JGI has sequenced many basal plants. They will sequence across them to assemble complex genomes.

Petsko asked what big questions the GTL would address. Weatherwax answered that it is desired to reengage the researchers to elicit big questions. The office is always encouraging people to address fundamental questions that will transform the science.

A break was declared at 3:19 p.m. The meeting was reconvened at 3:36 p.m.

Jeff Amthor was asked to present an update on the next-generation ecosystem experiment.

In the past few decades, BER developed and implemented leading technologies and approaches for the large-scale, long-term experimental study of the potential effects of climatic change on terrestrial ecosystems, including successful implementation of and leadership in ecosystem-scale (FACE) and precipitation manipulations. Now, the question is, what and where are the critical ecosystem research needs?

The Office has been engaged in an ongoing series of discussions with BERAC. They have held a Workshop on Exploring Science Needs for the Next Generation of Climate Change and Elevated CO₂ Experiments in Terrestrial Ecosystems in 2008 and a workshop on Identifying Outstanding Grand Challenges in Climate Change Research: Guiding DOE's Strategic Planning in 2008. There was also the *Report of the BERAC Subcommittee Reviewing the FACE and OTC Elevated CO₂ Projects in DOE* in 2006.

High-level criteria were developed by the BER staff, stating that the next-generation ecosystem-climatic change experiments should be (1) in ecosystems that are globally important with respect to potential feedbacks to climatic change, including the potential for significant effects on carbon cycle, surface albedo or sensible-energy exchange, and hydrologic cycle; (2) in ecosystems that are expected to be sensitive to climatic change, such as those where temperature or precipitation are critical constraints or are near environmental thresholds; (3) with ecosystem-climatic change combinations that have been relatively understudied (e.g., tropical systems, high-latitude systems, or complicated/complex systems) in order to fill larger knowledge gaps; and in locations and using technology that make the experiments feasible with expected resources.

A focused one-day meeting was hosted in February 2009 of seven national laboratory scientists with unique expertise in long-term, large-scale ecosystem-climatic change field experiments. The discussion concluded that (1) DOE priorities include multi-factor experiments (warming in combination with elevated CO₂) in intact ecosystems and (2) the priority ecosystems were tropical forest, tropical savanna, boreal forest, and arctic tundra with the last looking feasible in the near term.

Some carbon stocks of importance are the preindustrial atmosphere with 594 Pg of carbon, the present atmosphere with 820 Pg, global soil with 2050 Pg, and the northern permafrost region to a 3-m depth with 1672 Pg.

The short vegetation of arctic tundra may make it amenable to the next-generation experiment, but the arctic environment would pose challenges:

- High-latitude permafrost contains large stocks of carbon.
- Past, present, and future warming is greatest at high latitude.
- Warming increases the active layer depth layer and melts permafrost, which could cause a large release of CO₂ and/or CH₄ to the atmosphere.
- Warming will reduce the albedo (another positive feedback).

BP is monitoring the active layer depth at Prudhoe Bay; for the period 2005–2008, active layer thickness increased. From 1993 through 2008 there was a clear increase in temperature at depths from 20 to 55 meters. While soil at those depths is still solidly frozen, the warming trend is rapid: +1.3 °C in 12 years at 20 m. Deep-soil (20-m) warming is greatest at the northernmost sites, but may be occurring generally across northern Alaska. In simulations based on the A1B emissions scenario of the Intergovernmental Panel on Climate Change (IPCC), within about 50 years, permafrost at 1 m depth becomes summer water. By year 2100, about 80% of “near-surface permafrost” is lost.

A one-day workshop was hosted in July 2009 for persons conducting ecological research in arctic tundra. The purpose was to discuss a potential arctic tundra warming/elevated CO₂ experiment. Such an experiment could be built around the high-level question, what is the overall climatic change feedback potential of the arctic? The workshop concluded that

- A wide range of temperature and CO₂ values should be used to understand nonlinear and potential “threshold” responses to climatic change.
- Good replication is needed, and where to do the experiment is an important question.
- Active layer thickness would be a key variable and possibly the best measure/integrator of the temperature treatment.
- Modeling would be critical before, during, and after the experiment.
- A full range of ecosystem processes should be studied.
- Novel techniques will be needed for measurements, access to experimental plots, and modeling.
- Wide community participation should be facilitated.

Proposed questions to be addressed include

- What are the most critical science questions about effects of climatic change in arctic ecosystems?
- How can the next-generation arctic climate change experiment best answer those questions?
- What critical lessons can be learned from ongoing (and past) studies in designing the next-generation experiments?
- What are the key technological requirements for future research?
- How can the next-generation experiment best complement other arctic research, both experimental and observational?

There are at least three general approaches to a controlled warming and elevated-CO₂ experiment in a short-statured terrestrial ecosystem: an open-air approach, controlled-environment field chambers, and an in situ or off-site mesocosm arrangement. The field chamber approach to controlled warming differs from the “passive heating” approach now used in high-latitude research. Present systems are based on the “real” greenhouse

effect, and lack fine temperature control. The first two approaches would require new approaches to deep soil warming. Combining infrared lamps for surface (vegetation) warming with FACE for CO₂ enrichment can provide a completely open-air experiment, and the stature of arctic tundra would be amenable to such a combination. Study of the critical belowground environment would, however, require independent soil warming technology not yet proven in the field.

Field chambers are well-tested means to control CO₂ and temperature. Mesocosms are effective in maintaining above- and belowground environmental control for short vegetation both indoors and outdoors. Each approach has pros and cons. It must be determined which approach should be used going forward and which question(s) each would be able to answer.

Significant infrastructural support will be needed for any large-scale warming and elevated- CO₂ experiment, including large amounts of reliable power, reliable clean CO₂, and site access and protection (from bears).

Prudhoe Bay and Barrow were toured to explore potential access and support infrastructure and concluded that warming belowground permafrost in situ without causing a physical “mess” will be a technological challenge.

Preliminary design has begun on potential approaches for warming several meters of soil. Prototype development and testing should begin soon. Detailed 3-D heat-transfer modeling in permafrost is being applied to understand where and how much heat should be added to an arctic soil. Fluid dynamics modeling of aboveground heat and CO₂ transport is being conducted to evaluate various open-air or chambered systems in northern Alaska.

QUESTIONS/COMMENTS

Fowler asked what was known about the tundras. Amthor replied that they are now frozen and not doing anything. When they melt, the microbial community will produce CO₂ and CH₄, but it is not known in what ratio those gases will be produced. Tiedje noted that, in some regions, there is already a lot of methane produced.

Fowler asked how the active layer was defined. Amthor replied that the active layer is how far down the tundra melts by the end of the summer.

Petsko asked when this experiment would be over. Amthor said that a 10-year program was being talked about; that would include 10 freeze/thaw cycles.

Ehleringer asked Amthor if he realized how much thawing had happened since 2006. The time to do this research is now, not the future. When the tundra thaws, it is not just a climate problem but a hydrologic and microbial research question. By the time one gets around to doing this research, the thawing will have already occurred. Amthor agreed that warming is the big driver here. New approaches are needed. New money is not in hand for this research. The FACE experiments need to be concluded to free up money. This problem really *is* pressing. Ehleringer stated that a national scale of enthusiasm needs to be whipped up. Amthor noted that a workshop of multiple agencies is being held in a couple of weeks.

Tiedje pointed out that this is a major national-security problem and should be addressed by multiple agencies.

Stacey asked if models had taken these facts and feedbacks into consideration. Randall answered that these processes have not been forgotten, but this area is not in a

state of mature scientific understanding. Amthor said that present models do not have permafrost carbon in them.

Zhang asked how the carbon got there. Amthor said that it is 10,000-year-old windblown sediment.

Washington noted that the first calculations of the permafrost carbon release did not get the active zone right. Now, a good job is done in capturing the carbon release from the active layer. The projections of release from deeper permafrosts are scary. The 20th century is pretty well known, and the models need to be applied to the future.

Sayler noted that this research is a great opportunity to ask some terrific ecological questions that are not being addressed (e.g., susceptibility to invasive species). The problem should be looked at in an integrated manner. Amthor said that the plan is to have a broad archival approach, looking at a wide range of ecological variables.

Wildung asked why, if one has such a rapid change and needs such a wide-ranging ecological program, one should worry about controlled experiments. Why not just observe it as a natural experimental system? Amthor said that the question is whether what is going on now is going to be what goes on 100 years from now. The 10-year experiment would include ambient plots.

Palmisano said that the ecosystem approach may allow some leveraging of funds from sources outside the CESD, both within the BER and outside DOE.

Allison Campbell was asked to review the activities of the EMSL.

From FY06 to FY09, research at EMSL produced more than 1400 peer-reviewed publications and supplied 41 journal covers, 47% of its user proposals were funded by DOE and 13% by BER, 50% of its users were from academia from 26 countries and 47 states.

Under the advice of its Science Advisory Committee, BER, and the User Committee, the user program is focused on three science themes:

- Biological interactions and dynamics has five thrust areas: dynamics, composition and localization of cellular macromolecular complexes; protein modifications and how they impact cell regulatory networks; molecular mechanisms that define and control interactions between and within prokaryotic and eukaryotic cell communities; understanding phenotypic heterogeneity in cell populations; and characterizing and linking inter- and intracellular regulatory networks from the cell to the population level.
- Geochemistry/bigeochemistry and subsurface science has five thrust areas: linking molecular-scale processes to reactive transport; the interplay between geochemistry and the structure and activities of microbial communities; biogeochemical transformations of organic contaminants and natural organic matter (based on an understanding of radionuclide transport); nano-sensing for in situ characterization; and chemical and biological interactions at complex interfaces.
- The science of interfacial phenomena has three thrust areas: nucleation and growth in multiphase and multi-component systems (aerosols, biotic materials, etc.); phase separation and transformation; and charge and mass transport processes at interfaces that influence chemical transformations (particularly energy production or storage).

Proposals are submitted for participation in one of six modes: (1) partner (which entails cost sharing and capability building and can be entered at any time), (2) rapid (which lasts for up to 1 month and can be submitted at any time), (3) general (which lasts for up to 1 year and can be submitted at any time), (4) computationally intensive (which is responsive to a science-theme call), (5) capability based (which is responsive to a specific proposal call and can last up to 2 years), and (6) science theme (which is responsive to a specific proposal call and can last up to 3 years without resubmission). Science-theme proposals have taken off and have proven to produce more timely publication of results.

EMSL capabilities include molecular science computing, deposition and microfabrication, mass spectrometry, microscopy, spectroscopy and diffraction, NMR and EPR, surface flow and transport, and cell isolation and systems analysis. EMSL science is well aligned with BER programs and addresses national problems. EMSL also supports missions across DOE and other government agencies.

The ARRA was a game changer. The \$60 million investment funded approximately 30 instruments, of which 66% were purchased and 34% were EMSL built and of which 58% were new and 42% were upgrades. ARRA investments in microscopy will push the limits of resolution and allow in situ observation under real-time dynamic conditions, allowing atomic high-resolution of complex materials, extremely high spatial resolution, and unprecedented depth of field. ARRA investments in imaging will enable volumetric and nanoscale imaging of complex systems, giving 3D tomography/visualization for spatial and volumetric resolution in mixed media, nanoscale resolution for chemical and structural analysis of surfaces and interfaces, spatial analysis and localization of proteins etc., and unique ion contrasts that yield information about materials not otherwise available. ARRA investments will greatly enhance EMSL's world-leading capability in mass spectrometry, providing a 15-tesla Fourier-transform ion cyclotron resonance (FT-ICR) mass-spectrometry system, next-generation metabolomics characterization, an advanced mass-spectrometry capability, an ion mobility spectrometry-mass spectrometry proteomic system, an isotopic mass spectrometry capability, and a metabolomics capability. ARRA investments will greatly enhance EMSL's world-leading capability in magnetic resonance, giving EMSL the first 850-MHz wideband NMR system in North America, NMR console upgrades, a second-generation (multinuclear) bio-reactor/biofilm and in situ catalysis probe, a cryogenic magic-angle spinning probe, and the most modern and demanding pulse sequences for NMR users. ARRA investments will build a world-class interfacial molecular science capability for the study of radionuclides in environmental research with a 750-MHz wideband NMR system (the highest in the world for radiological samples), a focused ion-beam scanning electron microscope, a high-sensitivity X-ray photoelectron spectrometer, and a field-emission electron microprobe. Two other ARRA investments are a new computer cluster and archive storage. These ARRA investments have already led to new science.

EMSL is purchasing several major items of equipment (MIEs) in FY10: a high spatial resolution imaging secondary ion mass spectrometer (NanoSIMS), a high-resolution and -mass-accuracy capability project, and oxygen-plasma/ozone-assisted molecular-beam epitaxy.

Because petabytes of data are being produced from different experimental platforms and because of the need to move to real-time analysis, a portal is being developed to

manage those data. That portal, MyEMSL, will provide an end-to-end solution for users and their data.

Planned facility enhancements include

- A Radiological Capability that is awaiting CD1 approval to house four ARRA instruments and realize a BERAC recommendation from the 2005 review;
- A Quiet Wing that will have six vibration- and electromagnetically-quiet laboratory spaces, groundbreaking in December 2010, and four ARRA instruments; and
- The South Central Power Plant, which will provide the power and cooling needed for next-generation computing.

The next thing for EMSL is to fulfill Secretary Chu's bold vision to deliver transformational, breakthrough research; embrace a greater degree of risk-taking in research; pursue broader, more effective collaborations; partner globally; and improve connections among DOE, academia, and the private sector. It will do this with a global and national focus on energy, climate, and environmental challenges, employing ARRA and other capital investment. EMSL already has a solid foundation in its current science focus and operations. The path forward is to

- Refocus EMSL science themes (already accomplished);
- Assemble teams to find opportunities where molecular science can have a major impact, identify new approaches to accelerating science, define science and technology challenges and opportunities, identify capability needs/gaps, and develop resource needs/plan; and
- Vet team results with EMSL science and user advisory committees and with BER and to downselect and implement.

When this process is realized, EMSL will have contributed to the acceleration of discoveries that address DOE and global needs, demonstrated the power of multidisciplinary research, built a new generation of tools that push the limits of our users' imaginations, and enabled the seamless collaboration of research across space and time.

QUESTIONS/COMMENTS

Gilna asked if the new cornucopia of capabilities puts a stress on the facility's human capital. Campbell replied that it does, but that stress was planned for. New expertise is being sought, and attrition is being used to phase out older expertise. The facility has been working closely with BER.

Sayler asked if the characterization of organic matter included proteins etc. Campbell replied, yes.

Tiedje asked about the metabolomics facilities purchased and how they might contribute to the problem of genes of unknown function. Campbell replied that EMSL was trying to couple NMR to mass spectrometry in a realistic way.

Joachimiak asked, with so many technologies, how one stays state-of-the-art. Campbell admitted that one cannot. One needs to keep up to the state of the art in some areas and to be second in others. One listens to one's users and tries to respond to their needs.

Palmisano thanked Paul Bayer for his hard work in managing the ARRA funding.

The floor was opened to public comment. There being none, the meeting was adjourned for the day at 5:25 p.m.

Wednesday, February 24, 2010

Before the meeting reconvened, the Committee members were given their annual ethics briefing by a number of the DOE General Counsel's Office. The meeting was called to order at 8:33 a.m.

Wanda Ferrell was asked to give an overview of the new Atmospheric Systems Research (ASR) Program, resulting from the combination of the Aerosol Science and Atmospheric Radiation Measurement programs. It focuses on process research needed to improve the representation of clouds and aerosols in the climate models. New ACRF instruments open new research opportunities for ASR. Program managers Kiran Alapaty and Ashley Williamson have formed a team with the ACRF program managers, Wanda Ferrell and Rick Petty. The development of the Science Plan was driven by the new organization and the expansion of the number of instruments, which was made possible by the ARRA.

The goal of ASR, in partnership with the enhanced ACRF, is to quantify the interactions among aerosols, clouds, precipitation, radiation, dynamics, and thermodynamics to improve fundamental process-level understanding, with the ultimate goal to reduce the uncertainty in global and regional climate simulations and projections. Another goal is to supplement the long-term datasets with laboratory studies and shorter-duration field campaigns, both ground-based and airborne, to target specific atmospheric processes under a diversity of locations and atmospheric conditions. These projects are competitive. All of these data (long-term and campaign) are used together with models, to understand and parameterize the processes that govern the atmospheric components and their interactions over all pertinent scales.

Some of the important atmospheric processes are aerosol coagulation, chemical reactions, nucleation, condensation, radiation emission, turbulence, and convection. The community is recognizing these processes as a single system, and the new program reflects this integration of clouds, aerosols, and thermodynamics. The formulation of the working groups is just starting.

The ASR program will address the uncertainties in modeling the various processes in the aerosol-cloud-precipitation continuum. ASR's strategy towards characterizing this continuum in order to improve climate simulations is based upon a well-conceived suite of state-of-the-art instrumentation, measurement techniques, and experiments that are designed to observe fundamental aspects of the climate system at a variety of key locations. These observations target time scales ranging from rapid processes, through the diurnal evolution of the system, to seasonal and interannual variability of climatic conditions. Synergetic, multi-instrument methods are used to derive a comprehensive set of geophysical parameters that inform our process-level understanding, thereby providing the foundation for model development. Detailed process models are used to test and verify our physical understanding and, in turn, are essential for translating the results from local measurements to the much larger scales of climate models. Lastly, climate

model simulations are evaluated against measurements and derived geophysical properties.

The overarching objectives for the process research are (1) to determine the properties of, and interactions among, aerosols, clouds, precipitation, and radiation that are most critical to understand in order to improve their representation in climate models; (2) to ascertain the roles of atmospheric dynamics, thermodynamic structure, radiation, surface properties, and chemical and microphysical processes in the life cycles of aerosols and clouds, and develop and evaluate models of these processes; and (3) to identify and quantify processes along the aerosol-cloud-precipitation continuum that affect the radiative fluxes at the surface and top of the atmosphere and the radiative and latent heating rate profiles. The new instrumentation will support a lot of this research.

Observational and process modeling activities are intimately linked. Model studies and uncertainties establish observational priorities by specifically identifying the geophysical parameters and processes that must be better understood. In turn, observational data sets are used to initialize, constrain, evaluate, develop model parameterizations, and accelerate the improvement of the model.

One of the strengths of ASR is the strong relationship between observers and modelers, which will allow the development of research strategies to create the integrated data products necessary to improve the understanding of aerosol-cloud-radiation-precipitation interactions (e.g., retrieval development, uncertainty analysis, data product collation, and quality control).

Measurement and process modeling research will employ aerosol, cloud, precipitation, radiation, and dynamics and thermodynamics observations that will look at new-particle formation, liquid or ice formation on an aerosol, secondary organic aerosols, aerosol microphysics and optical properties, amount of condensed cloud water, cloud particle sizes, mixed-phase clouds, the precipitation field, droplet sizes, spectral shortwave radiative transfer, optical depth, relative humidity, cloud-scale dynamics, and surface latent and sensible heat fluxes. Precipitation radar will be added to all fixed sites.

The modeling side will look at atmospheric convection, large-scale forcing data sets, flexible frameworks, and different space and time scales.

The last part of the plan looks to the future and the recommendation of climatic locations that need further investigation (i.e., with either fixed ACRF sites or AMF deployments). There was also some consideration of expansion of the aerial facility for better sampling of the modes of variability and for the development of new in situ instrumentation to measure variables not measured or not well measured. To do that, it may be necessary to develop new remote sensing capabilities to measure geophysical variables that are currently only made in situ or not at all. The program does not do instrument development but may do “maturation studies.”

QUESTIONS/COMMENTS

Penner noted that one has the aerosol lifecycle, the cloud lifecycle, and cloud-aerosol interactions and asked what the distribution of funding was. Ferrell replied that this will be determined by the responses to the solicitations. There will be balance. Penner noted that there is often overlap of these areas in models and in research and asked how such proposals will be evaluated. Ferrell replied that the decisions will be made by all the program managers.

Sayler asked what radiation was being talked about. Ferrell answered: incoming solar's mid-spectrum. There will not be a mid-latitude observatory.

Mace stated that ASR is an observational campaign. There has not been a flow-through to the modeling community. Ferrell replied that that flow-through is what is trying to be accomplished.

Wildung said that, if one runs a model, one must have identified some critical areas to address and asked if that had been done to guide the research. Ferrell answered that, if one wants to improve a model, one has to improve the physics in the model. One needs observations to define the physics. It is an iterative process. Zhang noted that this has been done in looking at how clouds change as the climate changes.

Leung stated that the mobile facility has been useful and asked how much money goes to infrastructure versus research. Ferrell replied that she did not have the statistics with her. Long-term data are collected, and long-term campaigns are conducted. It cost \$2 million to deploy the mobile facility. Sometimes other agencies use it, so they contribute, but the expenditures that they make are not tracked by DOE.

Michael Kuperberg was asked to describe the Climate Research Road Mapping Workshop.

Generally, other workshops have been focused on a specific research topic. It needs to be determined how to pull all these research topics together. This workshop will provide guidance from the community on how to do that.

This effort can build on such prior documents as the DOE Climate Change Research Program's strategic plan of 2008; the Atmospheric System Research science plan of 2010; the ARM Climate Research Facility workshop report of 2009; the Integrated Assessment workshop of 2009; BERAC reports; the climate grand challenges of 2008; reviews of the ARM program in 2007, FACE facilities in 2006, integrated assessment in 2007, and climate modeling in 2008; National Academy of Sciences/National Research Council reports; U.S. Global Climate Research Program syntheses and assessment products; and IPCC assessment reports.

It is believed that the big questions are known. The question is how to put the information together, ensuring that atmospheric-process research, observations, climate-modeling research, integrated-assessment research, and terrestrial-process research are coordinated and connected.

The workshop approach will be to roadmap climate research, particularly in the areas of unique DOE strengths in atmospheric sciences, terrestrial ecosystems, and climate modeling. The goal is a concise research roadmap to inform BER's climate science program over the next 10 years. The document is intended for DOE leadership, informed nonexperts. The emphasis will be on disciplinary interfaces. Breakout groups will look at knowledge gaps and opportunities across latitudinal gradients and across temporal and spatial ranges.

There is an external steering committee and an internal committee. Two full days of meeting are anticipated with about 50 invited participants plus DOE staff. White papers are being developed by the steering committee with small writing teams to inform the workshop discussions.

QUESTIONS/COMMENTS

Zhang asked what the difference would be from BERAC. Kuperberg replied that the meeting on the following week and the grand challenge workshop are general, out-of-the-box, and long term. Specific guidance for the short term is needed.

Wildung asked if there are subtopics in clouds that are critical. Also, where is the real focus of this research, and what are the real scientific goals? How are you going to roadmap research that does not have defined goals? Kuperberg said that 5- and 10-year outcomes are being looked for. The gap between observers and modelers needs to be bridged. The discrepancies between model projections and accumulated data need to be reduced. Wildung asked if the workshop would focus on research goals. Kuperberg said it would, and those goals are being developed now. Palmisano added that these goals have been developed in a variety of ways in the past, and how to reach those goals needs to be planned.

Washington cautioned that the computing side needs to be brought in. Kuperberg agreed. BER works with ASCR on that. However, BER does not have a definite “customer” as the “recipient” of its research.

A break was declared at 9:25 a.m. The meeting was reconvened at 9:46 a.m.

Daniel Rothman (Department of Earth, Atmospheric, and Planetary Sciences, MIT) was introduced to discuss disordered kinetics in Earth’s carbon cycle.

Complex systems both display variability and structure, extreme events and/or non-Gaussian fluctuations, emergence of complexity from simple interactions, and a tendency to exist in marginally stable states. Studies of such systems emphasize commonality. Universality exists when qualitative characteristics determine quantitative behavior. In real-world systems, true universality is rare. Instead, one studies exemplary systems (pseudouniversality) to learn lessons of wide applicability.

The carbon cycle describes the transport and transformation of carbon as it cycles through living organisms and the physical environment. This talk focuses on rates of decay of organic matter—the rates at which organic carbon is converted to CO₂. These rates are disordered, but some have some structure: some are “fast” but most are “slow.” What is sought is the origin of these disordered rates; a quantitative understanding of them; and how they influence the carbon cycle.

The carbon cycle is a balance between photosynthesis and respiration. CO₂ concentration falls with increased photosynthesis. CO₂ concentration rises with increased respiration.

At the geologic time scale, other processes like inorganic-carbon burial prevail. Fluxes of CO₂ to the atmosphere are respiration (the fastest), combustion, and volcanism.

Respiration rates matter because, as tundra warms, microbial respiration increases.

But predictions are hard to make. One can couple carbon-cycle models with climate models. Results from 11 coupled climate–carbon-cycle models are very scattered. One century’s worth of scatter in the carbon uptake rate is roughly equivalent to the atmospheric reservoir of CO₂.

Despite the complexity of the situation, if one collects data, the processes seem to be straightforward. For example, the metabolic theory of the environment presumes a metabolic rate, production, and respiration, which suggests a production rate/respiration rate ratio of about $\exp(0.3 \text{ eV}/k_B T)$. In practical terms, as T changes, the increase in the respiration rate outpaces the increase in production.

Marine respiration rates decrease with age of the organic matter. Similar measurements exist on land, also. The decay curve shows a simple (linear power law) decrease in the respiration rate with time. A similar aging effect is observed in soils.

Possible origins of the aging effect include the chemical explanation. Organic matter is chemically heterogeneous, and fast reactions precede slow reactions. Another way to look at it is the physics explanation: Decay likely involves some kind of reaction-diffusion process. In structured environments (e.g., sediment), long diffusion times might imply slow rates. A statistical approach would say that decay represents an average of many simultaneous relaxation processes. Variability in the rates may suffice for the slowdown. A strictly mathematical approach would suppose the bulk decay $g(t)$ to be proportional to t^{-a} . Then $K(t) \equiv -d \ln g/dt = a/t$; and the “effective reaction order” is $1 + 1/a$ (which is too formal to be satisfying).

An example is degradation of forest litter. Litter is collected in litter bags, and the contents are sampled and analyzed annually for, say, 10 years. If one assumes first-order kinetics, then the rate would be an exponential. But the litter decay is not the straight line one would expect from an exponential process. “Multi-exponential” models explain the results by presuming multiple decay rates that depend on moisture availability, litter type, temperature, etc.

A different perspective, disordered kinetics, assumes that a continuum of rates k contribute to decay and that these rates are effectively random, drawn from an unknown probability distribution, each producing an exponential decay. This random-rate model of parallel relaxation produces an average (static) rate.

Static disorder is a reasonable approximation when the dry mass of carbon over time is a “completely monotone” and the exchange between different “pools” is slow compared to decay.

In the application of such an approach, a small error in the rate will produce a large error in model results.

For one litter bag, $p(\log k)$ is Gaussian, but $p(k)$ is log-normal. If one looks at hundreds of litter bags, they are all log-normal. Taking 232 datasets from 25 forests and plotting their log-normal parameters, the whole scatterplot looks like a mess, but some samples just have one rate and produce a straight line. The others exhibit disorder. In general, $\mu (= \ln k)$ increases with temperature and precipitation, and both μ and $\sigma [= \text{var}(\ln k)]$ increase with increasing nutrients. The variance of rate in log space increases linearly with the nutrient availability. This can be interpreted to mean that greater resources lead to greater diversity in rates and faster decay, which increases the average rate, also. Variability in rates (due to variability in substrate, environment, and decomposers) creates long-lived “slow” carbon pools.

Why are log-normal rate distributions so common? One would get a log-normal rate if one assumed that degradation occurs only after N distinct local conditions have been satisfied in sequence, each with an independent probability p_i of occurrence. Examples of such conditions include the water content, pH, nutrient concentration, microbial community, oxidizing agent, concentration and type of organic matter, etc. The probability P per unit time of a degradation “event” is $P = p_1 p_2 \dots p_N$, which means that $\ln P = \ln p_1 + \ln p_2 + \dots + \ln p_N$, and a sum of logs leads to a log-normal rate and log-normal rate distributions *should* be ubiquitous. They account for variations in chemical, biological, and physical parameters. A reinterpretation of our earlier study of sedimentary

organic carbon suggests that sequences of probabilities apply equally well at much longer time scales.

In sediments, microbes occur in voids surrounded by clay particles, suggesting that local reaction rates depend on the accessibility of organic matter to diffusing enzymes. So, if decay is limited by hydrolysis, then hydrolysis is limited by diffusion and the diffusion length over a typical enzyme “lifetime” is much less than the distance between microbes and decay would follow a random-rate model.

A worldwide database of sediment cores with 23 dated cores from varied sedimentary environments showed that log-normal rates apply equally well to long time scales in marine sediments. The slowdown of the instantaneous respiration rate also follows a log-normal path. Mineral dissolution rates slow down similarly, which implies that disordered micro-environments yield wide log-normal rate distributions.

For a steady production of organic matter, log-normal rate distributions predict that, as variance increases, reservoirs of stored carbon become much larger and much, much older. Therefore reservoir sizes (e.g., CO₂ levels) depend sensitively on the slowest rates. This has important implications on what issues are important.

Theoretical work on the carbon cycle and its impact on climate is mostly concerned with the construction of complex models, and predictive accuracy is of paramount importance.

Sometimes, one can replace a complex model with a log-normal distribution, but it does not immediately lead to more accurate predictions of the carbon cycle’s impact on climate. But, by expressing a vastly complex problem in terms of its overall heterogeneity, rather than trying to describe each aspect of that heterogeneity, we learn some important lessons of wide applicability. These lessons should ultimately lead to better predictions, but their immediate value is increased understanding. This increased understanding is the objective of “complex systems science.”

In conclusion, biogeochemical data can be transformed to a meaningful physical space, by assuming decay is a superposition of first-order processes and by inverting decay data for the distribution of rates. Such analyses reveal the universality of log-normal rate distributions and that their relation to the 1/t rate slowdown. Heterogeneity of environment, substrate, and biology produce diversity of rates (suggesting ecological diversity) and a sensitive dependence of carbon stocks on this diversity.

QUESTIONS/COMMENTS

Dickinson said that it would seem that identifying the rate-limiting factors would be important. Rothman replied, no. If one sums up a bunch of things, one gets a Gaussian distribution, but the factors do not have to have Gaussian distributions.

Wildung said that he kept looking for a stretched exponential. Rothman replied that that occurs in some situations but not all.

Joachimiak asked what was known of the chemistry of fast-decaying processes. Rothman responded that what is known is greater than what he knew. It comes down to the ability of enzymes to break down organic material. The average age of carbon in the ocean is 6000 years, but it is not known why.

Mace noted that Rothman had said that if one takes out any processes, it does not make any difference. Rothman answered that the suspicion was that something about the

disorder of the situation is important. There is a path to follow, but it is not known what is going on. That notwithstanding, you know what you can expect.

Wildung pointed out that there are 150 years of research on carbon aging and that it is generally accepted that many processes occur in a chain of events giving a chemical/microbial process. He asked if Rothman had any insights. Rothman replied that this is not the only way to address the problem. It has to be used in a complementary manner with other approaches.

David Lesmes was introduced to brief the Committee on the Subsurface Biogeochemical Research Program Workshop.

The BER mission is to understand complex biological, climatic, and environmental systems across spatial and temporal scales. The Subsurface program has an FY10 budget of \$50 million to advance a fundamental understanding of coupled physical, chemical, and biological processes controlling contaminant mobility in the environment. The challenge and overall approach are to conduct characterization and monitoring; investigate microbiology, geochemistry, and hydrology; perform modeling and high-performance computing; and operate molecular science, EMSL, and light sources in studies that range from the field scale to the macromolecular scale.

There is a network of university and national-laboratory collaborative projects leading to a highly multidisciplinary predictive understanding of subsurface processes. Field sites are funded at \$3 million per year for 5 years each.

A workshop was conducted in August 2009 to identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems. With the logic model format, a strategic plan is being developed for the BER contaminant fate and transport research program for a 10-year planning horizon. The logic of logic models starts with the end in mind. One then sets goals, going from the most general to the most specific until one reaches the current situation.

The workshop goal was to identify knowledge gaps and science challenges that must be met to predict contaminant behavior in complex subsurface systems. Its objectives were to define complex subsurface systems and establish why they are important to different DOE environmental and energy mission outcomes; to consider how the coupling of subsurface processes can be used; to evaluate research approaches that can be used to identify and account for the influence of smaller-scale processes and their mechanisms on larger-scale system behavior; to conceptualize the models needed to describe and predict complex system behavior at different scales; and to identify significant, long-term, interdisciplinary research opportunities associated with complex subsurface systems.

Complex systems were the subject of a lot of discussion at the workshop. It found that there are similar characteristics and attributes (emergent phenomena, intermittency, and coupling) across scales and asked if similar research approaches can be developed to advance the predictive understanding of complex-system behavior. However, each complex system is different. Apparently there are no general laws for complexity. Instead, one must look for rules that might be seen in one system and applied to another.

Complexity methods often use a top-down approach to identify key interactions controlling diagnostic variables at the prediction scale; general macroscopic laws controlling system-scale behavior; and simplified models of subsystem interactions that

enable prediction. This approach is analogous to the systems biology approach, which is defined as the holistic, multidisciplinary study of complex interactions that specify the function of an entire biological system rather than the reductionist study of individual components. Both approaches emphasize the tight coupling between experimentation and modeling.

One breakout session identified favorite complex systems by scale. A second breakout session identified key research priorities for investigating complex subsystems by discipline. Some key complex systems were extracted to address in a breakout session that defined complex subsurface system challenges and research goals across scales and disciplines.

The reductionist philosophy is that overall system behavior can be understood from a detailed understanding of the system components. The complexity philosophy is to seek to identify and understand commonalities between complex systems and their relationship to simpler systems. The reductionist strategy is to understand and model system behavior as some permutation of the sum of its lower scale parts – blame heterogeneity for shortcomings. The complexity strategy is to identify diagnostic variables and transferable macroscale laws that define or describe high-level system behavior. The reductionist research approach is bottom-up and mechanistic. The complexity research approach is top-down and phenomenological. Reductionist modeling employs mechanistic details of lower-scale processes that are preserved but streamlined in upscaling; models are calibrated to account for the effects of heterogeneities. Complexity modeling uses phenomenological models to explain and describe key processes' contributions, interactions, and properties that control system behavior.

It was recognized that a hybrid approach is needed, and the report calls for a pragmatic melding of bottom-up and top-down approaches. It emphasizes the identification and understanding of key underlying mechanisms and interactions and the importance of scale transitions, while simultaneously providing insights on common macroscopic laws governing complex system behavior at the prediction scale. The goal it sets is to achieve comprehensive and quantitative system predictability through iterative experimentation and modeling.

The heart of the report is the three groups of complex-system research opportunities:

1. Understanding fundamental subsurface process coupling
2. Identifying and quantifying scale transitions in hierarchical subsurface systems
3. Understanding integrated subsurface-system behavior

The challenges associated with the first group are coupled mineral-microbe interfacial processes, microbial community responses in dynamic subsurface conditions, quantifying biogeochemical rates in heterogeneous media, and feedbacks between biogeochemical transformations and flow. The challenges associated with the second group are identification of smaller-scale controlling variables and diagnostic signatures, measurement approaches for key variables and diagnostic signatures, and scale transition models. And the challenges associated with the third group are identification and simulation of field-scale emergent phenomena; observation, integration, and explanation of large-scale behavior; and phenomenological models for predicting dynamics at and above the plume scale.

The path forward is to apply a hybrid research approach to advance predictive understanding of hierarchical subsurface systems by combining complimentary bottom-

up reductionism with top-down complexity concepts through iterative experimentation and modeling. Well-conceived, hybrid research efforts at selected DOE-relevant field study sites and representative laboratory model systems at different scales offer the most potential for understanding fundamental process interactions that occur across scales and lead to complex subsurface behavior. The value of complex system science approaches in providing the scientific basis for effective DOE management of earth/environmental systems should be explored.

QUESTIONS/COMMENTS

Zhang noted that the program is focused on understanding processes, but he did not see the tie-in to predictive models. Lesmes pointed out that BER has two SciDAC projects on modeling and that one-third of its portfolio goes to developing predictive models. An open-source community model is funded for the next 5 years, leveraging BER's work during the past 15 years. That model is to go from the microbial to the field scales. The processes that are modeled need to be quantified.

Zavarin stated that the focus of the subsurface program is environmental-management issues, but the workshop report focuses on fundamental science. The subsurface science needs to be incorporated into climate research. He asked how projects are distributed between environmental management and fundamental science. Lesmes replied that a lot of the work being done to inform environmental management has a lot of commonality with climate science and modeling. Palmisano agreed. She pointed out that it also benefits others' work (e.g., work at EMSL and climate research done at other agencies). Lesmes said that the program could contribute to carbon cycle research, also. Principal investigator meetings might discuss carbon nutrients.

Hubbard stated that this workshop is focused on subsurface science that is applicable to a lot of DOE missions and offices, not just on environmental management issues.

Gary Stacey (BERAC) introduced the topic of the BER Grand Challenge Workshop. A steering committee set up subcommittees on

- Climate
- Sustainability
- Informational and synthetic biology
- Systems biology

Four position papers have been finalized and distributed to all workshop participants. This event has been described as a strategic planning workshop, but that is not to be its output. Rather, the purpose is to identify grand challenges to guide future BER research.

The charge letter calls for the workshop to address four questions:

1. What are the greatest scientific challenges in biology, climate, and the environment that DOE will be facing in the long term?
2. How should BER be positioned to address those challenges?
3. What new and innovative tools should be developed to advance BER science?
4. What scientific and technical advances are needed to train the workforce of the future in integrative science, including complex-system science.

The agenda has been set. A balance of seven stimulating talks has been struck with time for discussion. Breakout groups have been scheduled on climate change; systems biology; information and synthetic biology systems integration framework; research

framework for energy sustainability; understanding systems across temporal and spatial scales; meeting the workforce and education needs; data integration and knowledgebase development; and novel tools, techniques, and probes. A report will be made to the larger group, and a writing committee will produce a draft report in the three days following the meeting.

Hubbard asked how the four main topics were chosen. Stacey said that the discussions of the steering committee were distilled down, and then the steering committee wordsmithed the results, taking into account the wide ranging comments from a prior BERAC meeting. This workshop will identify many grand challenges across a broad range of topics. They will go to DOE to be used in selecting the topics of future, more selective workshops.

The floor was opened to public comment. **Peter Daum** asked who else was going to be represented at the workshop. Stacey said that this invitation-only workshop will not be open to just BERAC members but to a wide range of academics, national laboratory personnel, and disciplines.

There being no further public comments, the meeting was adjourned at 11:41 a.m.