

DRAFT
Minutes of the
Biological and Environmental Research Advisory Committee Meeting
September 1-2, 2009
Marriott Washingtonian Hotel, Gaithersburg, Md.

BERAC members present:

Gary Stacey, Chair
S. James Adelstein
Eugene W. Bierly
Janet Braam
Robert E. Dickinson
James R. Ehleringer
Joanna S. Fowler
Andrzej Joachimiak
Raymond F. Gesteland
David T. Kingsbury

Joyce E. Penner
Gregory Petsko (Tuesday only)
David A. Randall
Karin Remington
Margaret A. Riley
Gary Saylor
Judy Wall
Raymond E. Wildung
John C. Wooley

BERAC members absent:

Margaret S. Leinen
Stephen R. Padgette
James M. Tiedje

Warren M. Washington
Mavrik Zavarin

About 62 others were in attendance during the course of the two-day meeting.

Tuesday, September 1, 2009
Morning Session

Judy Wall joined BERAC as a new member.

Chairman **Gary Stacey** called the meeting to order at 9 a.m. He thanked and commended Michelle Broido for her service as the previous chair of the Committee. He had the members introduce themselves. He requested suggestions on how to better manage the Committee and urged the members to participate vigorously and make these meetings events of intellectual athleticism.

Patricia Dehmer was introduced and asked to provide an overview of the activities of the Office of Science (SC). She expressed an interest in normalizing the conduct of the SC advisory committees. All of the offices of SC should contribute to the three themes of SC [science for discovery; science for national need; and national scientific user facilities, the 21st century tools of science] and should recognize their contributions to all three themes.

Funding of SC programs in FY10 is led by Basic Energy Sciences (BES) at \$1.7 billion, followed by High-Energy Physics (HEP) at \$819 million and Biological and Environmental Research (BER) at \$604 million. SC funding goes to research, facility operations, facility construction, and major items of equipment (MIE). BER support is

still overwhelmingly dominated by research, one of the true strengths of the program; about one-quarter of its support goes to facility operations.

SC operates computational resources; synchrotron light sources; neutron sources; particle accelerators, colliders, and detectors; fusion/plasma facilities; the Nanoscale Science Research Centers (NSRCs); the Joint Genome Institute (JGI); the Environmental Molecular Science Laboratory (EMSL); and atmospheric and environmental facilities. BER facilities are different from those that SC is known for (e.g., the light sources).

SC will have about 25,000 users at its facilities in FY10, about one-half from universities and about one-third from national laboratories with the remainder from industry, other agencies, and international entities. BES facilities account for about one-half of SC's users; 17% of SC's facility funding goes to the light sources. BER accounts for about 2500 or 10% of SC's users at the JGI, EMSL, and Atmospheric Radiation Measurement (ARM) Climate Research Facility (ACRF).

SC also contributes to training the next generation of scientists and engineers, although at nowhere near the level of support provided by the National Science Foundation (NSF). In FY09, 4,400 grad students and 2,700 postdocs were supported by SC; ~550 undergraduates interned at DOE laboratories, ~280 K-16 educators trained at DOE laboratories; and 300,000 K-12 students, 21,000 educators, 3,000 graduate students, and 4,200 undergraduate students participated in DOE laboratory activities. The DOE National Science Bowl attracts ~22,000 high school and middle school students annually. SC initiated the Graduate Fellowship Program for steady-state support of 400 graduate students with American Recovery and Reinvestment Act (ARRA) funds and the FY10 request.

SC's ARRA projects totaled \$1.6 billion, which had to be allocated in a very short time. The ARRA goals are to preserve and create jobs and to spur technological advances in science and health. SC ARRA projects had to meet several principles: to be shovel-ready, enhance research infrastructure and support high-priority R&D, low risk (e.g., construction projects were baselined with in-place or imminent CD-3; research projects had proposals in hand or solicitations were to be fast), and creating no out-year mortgages [with two exceptions: the new Energy Frontier Research Centers (EFRCs) and the Graduate Fellowship/Early Career Awards]. The Early Career Awards will support several hundred researchers; 2200 letters of intent (LOIs) were submitted. The due date for proposals was the day this talk was presented. The Secretary is very supportive of this competitive award program. Sizeable amounts of SC's ARRA funds went into construction:

- Acceleration of ongoing line-item construction projects: \$338.2 million
- Acceleration of MIEs: \$171.1 million
- Upgrades to SC user facilities: \$391.0 million
- Laboratory general plant projects: \$129.6 million
- Scientific research: \$562.1 million

The DOE Energy Innovation Hubs were proposed by Secretary Chu in the FY10 budget request. He was extremely impressed with BER's Bioenergy Research Centers and used them as a model in envisioning the hubs. These hubs would have critical mission needs, would be led by a scientific leader, and would be largely under one roof. The owner would have budget authority. However, few grasped the concept, and it met

with confusion on the Hill. DOE hopes to have three hubs start in FY10 and the others later.

President Obama has reinforced President Bush's desire to double the budgets of research agencies over 10 years with 2006 being the base year for SC. 2006 was an interesting year for SC with a low budget request and an appropriation that was about the same as the request but lower than the previous year's appropriation. Some programs (e.g., HEP) got mauled, and some [e.g., Advanced Scientific Computing Research (ASCR)] were well on the doubling path. In 2010, the request follows the doubling path. The House and Senate marks took nips out of the President's request. The radiochemistry and imaging program was transferred to the Office of Nuclear Physics (NP) but not the funding. This proposed transfer has been appealed by DOE. This confusing situation could be resolved in conference committee.

Two new charges are being presented to BERAC: to assemble a Committee of Visitors (COV) to review the management processes of the BER Climate and Environmental Sciences Division and to help articulate a vision for the BER program for the coming years. BES has previously looked at the basic research needed to advance its programs and the new science that must be delivered. Grand science challenges should be nondisciplinary and not necessarily mission relevant, simply science for discovery: major national studies. The second charge from Brinkman will ask BERAC to translate this experience to BER. The advisory committee can have a huge influence on how this charge is developed.

The U.S. energy flow for 2008 as measured by the Energy Information Administration shows that the nation consumed 99 quads of energy, produced 74 quads domestically, and imported 33 quads. This is in sharp contrast to 1950, when the nation was energy independent. A more-detailed analysis for 2007 shows that the building sector, industrial sector, and transportation sector consumed 102 quads from a supply of 107 quads, 67% of which was produced domestically and 33% of which was imported. The largest energy source was petroleum, two-thirds of which was imported. Other major sources were coal, natural gas, nuclear power, and renewables. 40.5 quads of this primary energy went to electricity production, which is very lossy. 58.5 quads were wasted, largely in electricity and transport; 43.0 quads were actually used. These figures can be used to develop an energy strategy. End-use efficiency needs to be increased. The electricity sector must zero out emissions by fuel switching and by carbon capture, sequestration, and storage (CSS) along with an improved grid. This strategy should be supported by climate and environmental science (i.e., compelling climate models). This strategy underlies the selection of hubs and drives the thinking of the leadership of DOE and the country.

The National Academy of Sciences (NAS) published *America's Energy Future*, which was supported by SC funding. Brinkman, Chu, and two under secretaries were on this panel. Harold Shapiro summarized this report by saying, "One of the Committee's conclusions is that there is no technological 'silver bullet' at present that could transform the U.S. energy system through a substantial new source of clean and reasonably priced domestic energy. Instead, the transformation will require a balanced portfolio of existing (although perhaps modified) technologies, multiple new energy technologies, and new energy-efficiency and energy-use patterns. But a timely transformation of the energy system is unlikely to happen without finally adopting a strategic energy policy to guide

developments over the next decades. Long-term problems require long-term solutions, and only significant, deliberate, stable, integrated, consistent, and sustained actions will move us to a more secure and sustainable energy future.”

BER is an important player in this investment strategy.

Stacey asked if there were any changes in how the advisory committees will be looked at in the new administration. Dehmer replied that the new administration is coming in fresh. Brinkman wants them to drill down on the important issues. He is very engaged in advisory-committee activities. Stacey said that Broido had pointed out that there were coordinating meetings of SC advisory-committee chairs. Dehmer replied that the chairs have gotten together and gone up to the Hill to meet with congressmen and staff. They have never gotten together to discuss committee management and culture.

Sayler asked if DOE will do anything to increase the number of graduate students. Dehmer answered in the affirmative. The administration is interested in doing that, and DOE and SC are discussing how to do that and how to increase the number of technical degrees granted by community colleges.

Bierly asked how that differed from the Workforce Development Program. Dehmer responded that workforce development does undergraduate programs, K-12 teacher training, the DOE Science Bowl, etc. with a budget of about \$20 million. The Early Career Awards support professionals already in the field.

Fowler stated that new technologies and tools need to be developed and that behavior has to be influenced for it to lead to innovation. Dehmer answered that this is a multi-agency problem and is being worked on by several agencies.

Stacey asked how the hubs were progressing. Dehmer replied that DOE hopes to start with three hubs in FY10 and to increase that number in future years.

Wildung noted that DOE has been guided by missions and that the NSF and the National Institutes of Health (NIH) have done discovery science. Dehmer responded that one can impact a lot of missions with basic science, so it is needed to go beyond the energy technologies we have today. One has to force the future by innovative, revolutionary science today.

Petsko stated that the facilities are one of the jewels of DOE’s crown and should be continued.

Penner noted that the National Oceanographic and Atmospheric Administration (NOAA) is working hard to incorporate climate services. Dehmer answered that multiple (20) agencies have a role to play in climate science. This administration recognizes that climate science is necessary.

Bierly noted that a significant amount of work is being done on the social aspects of climate change and global warming. Only 7% of the United States population thinks that climate change is not happening, but they are a very vocal minority.

Sayler asked if there were any risks of a lack of support in the future. Dehmer replied, yes, especially with the accumulation of out-year deficits. It is believed that the President will continue his commitment to doubling the research agencies’ budgets. However, industry also needs to step up. But industry only supports what produces an economic return in the short term, so it cannot be relied on to fill the gap.

A break was declared at 10:16 a.m. The meeting was called back into session at 10:31 a.m. **Adam Rosenberg**, staff member, House Committee on Science and Technology,

announced that there will be a hearing during the following week at which Anna Palmisano, Ari Patrinos, and others will testify about the BER program.

Anna Palmisano was asked to comment on the state of BER. She welcomed the new chair and member, thanked Michelle Broido for her service and leadership, and thanked Joanne Corcoran for her support of meetings.

One of the most important themes is science for discovery: in understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales. BER is trying to revolutionize bioenergy production through transformational discoveries in biology; integrate climate theory, observation, experiment, and modeling; develop new capabilities for analyzing and managing data to predict and engineer biological systems; and provide the fundamental understanding of environmental sustainability and stewardship by predictive understanding across scales.

BER has three national scientific user facilities: the Joint Genome Institute (JGI) for analysis of complex genomic systems including microbial communities, plants, and ecosystems; the ACRF Facility fixed and mobile sites; and the Environmental Molecular Science Laboratory's (EMSL) new capabilities for studying dynamic processes of chemical reactions and in living systems.

In the conduct of science to meet the DOE mission and national needs, BER is supporting research needed to develop biofuels as a major secure national energy resource; exploring the potential effects of greenhouse gas emissions on Earth's climate and biosphere, and their implications for our energy future; predicting the fate and transport of DOE-relevant subsurface contaminants; and developing new tools to explore the interface of biological and physical sciences.

The FY10 budget totals for BER are almost the same as the FY09 appropriation (before the ARRA): The President's Budget Request was \$604,182,000, of which \$318,476,000 was for Biological Systems Science and \$285,706,000 was for Climate and Environmental Sciences. The House mark decreased Biological Systems Science by \$2 million and Climate and Environmental Sciences by \$5 million. The Senate mark provided full funding but moved nuclear medicine to the Office of Nuclear Physics (NP); that transfer is being appealed.

BER greatly benefited from ARRA funds. The ARM Program received \$60 million for capital investments in instrumentation and research infrastructure for the fixed and mobile ARM facilities. Capabilities will provide (1) 3-D measurements of cloud-scale dynamics, microphysics, and precipitation and (2) enhanced measurements of atmospheric aerosol composition and chemistry. This funding will advance BER's mission and decrease uncertainty in climate models.

The EMSL received \$60 million for more than 25 leading-edge experimental capabilities, including nuclear magnetic resonance spectrometers; mass spectrometers; molecular/microscopy imaging capabilities; and nano- and molecular-level characterization instruments. This will be a great boon to all users of this facility.

Other ARRA investments include the Bioenergy Research Centers Capital Equipment expenditures, with the Bioenergy Science Center (BESC) at Oak Ridge National Laboratory (ORNL) receiving \$5.4 million, the Great Lakes Bioenergy Research Center (GLBRC) at the University of Wisconsin receiving \$4.1 million, the Joint BioEnergy Institute (JBEI) receiving \$4 million, and infrastructure for plant feedstock genome

analysis and characterization receiving support. The Integrated Assessment (IA) Research Program received \$4.9 million for computational and data storage equipment at the Pacific Northwest National Laboratory (PNNL)/Joint Global Change Research Institute. The JGI received \$13.1 million for infrastructure for genome sequencing, analysis and characterization for plant feedstocks at Lawrence Berkeley National Laboratory (LBNL). And ORNL received \$3.2 million for conceptual design and planning for a Systems Biology Knowledgebase.

The goal of the Early Career Awards is to train the next generation of young scientists at universities and national laboratories. 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 Biological Systems Science Division (BSSD) and Bob Vellario for the Climate and Environmental Sciences Division (CESD). These awards are high-profile projects and a passion of the Secretary. Early career is defined as on a permanent career track at an academic institution or national laboratory and no more than 10 years past the PhD. BER will fund eight awards in FY10; it has received 427 letters of intent in subsurface science (30); carbon cycle and ecology (63); atmospheric sciences (26); modeling (40); genomics (120); radiological sciences (12); computational biosciences (20); ethical, legal, and societal issues (25); and other (107).

BER is very active in interagency interactions, such as the U.S. Global Climate Change Research Program (made up of 13 agencies) in which BER is having discussions with NOAA about its National Climate Service. BER has been a long-time supporter of the Ameriflux network, participates in a joint program with the U.S. Department of Agriculture (USDA) on plant feedstock genomics, with seven other agencies has belonged to the Metabolic Engineering Interagency Program for 11 years now, operates the Protein Data Bank with NIH and NSF, researches the effects of low-dose radiation with the National Aeronautics and Space Administration (NASA), collaborates on structural biology with NIH's National Center for Research Resources and NSF, and is a member of the U.S.–European Commission Biotechnology Task Force. The mission of that Task Force is “To promote information exchange and coordination between biotechnology research programs funded by the European Commission and the United States government.” Its participants are the European Commission Research Directorate and U.S. agencies [NSF, USDA, DOE, Department of Defense (DOD), NIH, Environmental Protection Agency (EPA), Food and Drug Administration (FDA), National Institute of Standards and Technology (NIST), Office of Science and Technology Policy (OSTP), and others]. The Task Force will celebrate its 20th anniversary in June 2010. BER co-chairs the Working Group on Environmental Biotechnology and the Working Group on Biobased Materials and Bioenergy. Activities include jointly funded workshops, short courses, and fellowships.

BER is developing strategic plans for its core research activities. Plans have been completed for the programs to provide the foundational science needed to develop biofuels as a major secure national energy resource and to understand the potential effects of greenhouse-gas emissions on Earth's climate and biosphere and their implications for our energy future. It is in the process of developing a plan for research to predict the fate and transport of DOE-relevant subsurface contaminants and for research to develop new tools to explore the interface of biological and physical sciences.

In pursuit of these mission priorities, several workshops have been held this year. One looked at subsurface complex-system science relevant to contaminant fate and transport. This workshop included 36 scientists with research experience in the molecular to pore scale, intermediate scale, and field scale in the broad disciplines of microbiology, geochemistry, and transport modeling. The goal is to chart a path to a predictive understanding of subsurface processes that influence contaminant transport across scales in the environment.

In the Office, Roger Dahlman retired after 32 years at DOE. BER is looking for an ecologist to replace him. Renu Joseph has joined BER as an Intergovernmental Personnel Act (IPA) detailee in regional climate modeling. Cathy Ronning has joined BER as Program Manager in plant biology and genomics. Peter Kirchner will complete his BER detail and retire on September 30. Leslie Runion was promoted from secretary to administrative specialist; a CESD secretary is being recruited to replace her. A Science Assistant is being recruited for the BSSD. And a request to fill the CESD Director slot for CESD has been signed by Dr. Brinkman but needs even higher approval.

BER held a science retreat in June 2009. It focused on high-risk/high-reward research and science integration (how to link science in BER across BER programs, with other offices' science activities and with the activities of the technology offices).

A long-term vision is being developed by BERAC and will be included in a new charge to the Committee. Another charge will call for a COV for CESD. A JGI strategic planning document is in draft copy.

Bierly asked what some of the suggestions were for increasing high-risk/high-reward research. Palmisano answered that workshops should involve young and new investigators. High-risk/high-reward research should be encouraged. Money should be made available for proof-of-principle research. Peer review panels should be asked to consider high-risk/high-reward proposals. Additional ideas from BERAC would be welcome.

Dickinson asked about the status of coordination with other agencies on climate-change research. Palmisano replied that Shirley Abbot of OSTP has spoken with the U.S. Global Change Research Program (USGCRP). BER will be briefing her later this month. That Office supports interagency cooperation.

Adelstein asked how the BER was going to deal with all the Early Career Award applicants. Palmisano responded that peer-review panels will pick the very top people. SC was surprised by the huge response. Eligible applicants not receiving awards this year can reapply next year.

Sayler asked if the overall budget was affected by earmarks. Palmisano replied that the Office focuses on the presidential request and what comes out of it. It honors what requests or directives are received. Thomassen noted that earmarks are not shown in the BER budget; they are separate and included at the SC level.

Sayler asked how SBIR awards are handled. Palmisano answered that they are handled by an SC office, and BER coordinates with that office on issues of interest to BER.

Barbara Alving was introduced to discuss NIH's efforts to connect the nation's researchers, patients, and communities.

The NIH National Center for Research Resources (NCRR) translates research from basic discovery to improved patient care. It funds animal-model studies, preclinical research, clinical research, and community outreach through science education and community engagement. One of its largest programs is the Clinical and Translational Science Awards, whose goal is to ensure that new discoveries lead to improved public health. It encourages rapid implementation of biomedical discoveries; developing, testing, and bringing new prevention strategies into medical practice more rapidly; catalyzing change by lowering barriers between disciplines; and encouraging creative and innovative approaches.

NCRR has five strategic goals: to enhance

- National clinical research capability and efficiency through informatics and other means,
- Training and career development in clinical and translational science,
- Consortium-wide collaborations,
- The health of our communities and the nation through informatics and wireless technology, and
- T1 translational research (pushing biomedical discoveries toward preclinical trials).

NCRR is translating discoveries into tools for biomedical research through Biomedical Technology Research Centers (BTRC), which are reaching out to DOE; shared instrumentation; high-end instrumentation; investigator-initiated research grants; the Biomedical Informatics Research Network (BIRN); and small-business opportunities throughout NIH.

NCRR's Shared and High-End Instrumentation programs provide unique and critical NIH mechanisms, funding from \$100,000 to \$2.0 million, equipment that is too costly to obtain with regular NIH research grants, highly cost-effective mechanisms, and instruments for core facilities. These instruments are shared by an average of 8 to 10 grantees.

NCRR operates a shared biomedical information-technology (IT) infrastructure for collaboration between groups with different expertise and resources, shared infrastructure to support collaboration, and open access and dissemination of data and tools.

It provides support for 52 nationally accessible engines for translational research to train investigators as well as to serve a discovery function. These 52 BTRCs are classified in five broad areas with a scope that ranges from basic discovery to clinical research at a scale from the molecule to the organism. The areas of interest are imaging technology, informatics resources, optics and laser technology, technology for structural biology, and technology for systems biology.

NCRR interacts with DOE through its BTRCs located at DOE national laboratories in Systems Biology and Structural Biology (three are jointly supported with DOE/BER). NCRR Leverages Resources at DOE national laboratories to support NIH research, translating the results of research into tools. NCRR funds nine BTRCs at seven national laboratories to translate advances in physical sciences into tools for biomedical research. DOE national laboratories facilitate R&D that is expensive and complex and presents opportunities for NCRR to leverage unique expertise and infrastructure in the physical sciences. NCRR provides \$20 million to the national laboratories through personnel, instrumentation development, and instrumentation access. Examples are the National

Flow Cytometry Resource at Los Alamos National Laboratory (LANL), the National Resource for Biomedical Accelerator Mass Spectrometry at Lawrence Livermore National Laboratory (LLNL), and the Proteomics Research Resource for Integrative Biology at PNNL. The tools these cooperative efforts are producing include a simple, low-cost, compact data-acquisition system for compact, portable flow cytometers; the technology for the identification of chemoresistance for personalized chemotherapy; proteomics analysis to predict the process and outlook for trauma recovery.

The structural biology BTRCs at national laboratories include

- BioCARS: A Synchrotron Structural Biology Resource (ANL)
- Biophysics Collaborative Access Team (ANL)
- Undulator Resource for Structural Biology (ANL)
- Macromolecular Crystallography at the National Synchrotron Light Source (BNL)
- Synchrotron Radiation Structural Biology Resource (SLAC)
- National Center for X-Ray Tomography (LBNL)

At this point, more than 40% of all research done at DOE synchrotrons is in the life sciences. At the Stanford Synchrotron Radiation Laboratory (SSRL), a cooperatively funded program integrates three structural-biology technology-development areas to serve the needs of the biomedical and environmental science communities for macromolecular crystallography, X-ray absorption spectroscopy, and small-angle X-ray scattering. Most of the synchrotron work of Nobel Prize-winner Roger Kornberg was performed at SSRL and strongly enabled by the robotics. At the National Center for X-ray Tomography at LBNL, new technology obtains 3D views of whole, hydrated cells in their native state at better than 50-nm resolution. At the National Synchrotron Light Source-II (NSLS-II) at Brookhaven National Laboratory (BNL), beamlines for the life sciences are funded.

ARRA funds were used for instruments, research, and infrastructure:

- \$8.2 billion to extramural scientific research
- \$1.0 billion for extramural construction
- \$0.5 billion for intramural repair and improvement and construction
- \$0.3 billion for shared instrumentation and other capital equipment, and
- \$0.4 billion for comparative effectiveness research

What NCRR seeks to do is to maximize the investments made in NIH's grantees by collaboration with other agencies.

Stacey said that it was good to see such close cooperation.

Wildung asked if NIH had any separate mechanism for high-risk/high-reward research. Alving replied, no. NIH funds new-investigator awards. Investigators work closely with NIH facilities, and innovation is encouraged in other ways, such as training.

Petsko noted that NIH straddles the big-science/small-science fence and asked how that will play out in the next few years. Alving replied that NIH needs to go back and rethink how it allocates its core resources after it gets out from under the ARRA. It needs to change the dynamics to perhaps recognize depreciation and funding personnel and to bring in good business practices. Petsko stated that the best big science produces a lot of good little science. The NIH has grown toward the top-down setting of science priorities. It needs to incorporate some bottom-up priority setting that comes from and encourages small science. The trend toward big science is troubling. Alving replied that the problem is striking a balance. Funding opportunity announcements (FOAs) are, indeed, top-down

instruments. Within the centers, the funding should be used to foster creativity and innovation.

Horst Simon was introduced to describe future trends in computing.

The new NERSC-6 [National Energy Research Scientific Computing Center] system was just announced and will be named after Grace Hopper. It will be introduced in two phases. Phase 1 will have 668 nodes and 5344 cores; Phase 2 will have 6400 nodes and 153,600 cores.

ESnet will be upgraded to 50 to 60 Gbps between 2009 and 2010 and to 200 to 600 Gbps by 2012. It will be used to move climate-change data at a much greater rate. Key connections will be upgraded to 100 Gbps with \$61 million of ARRA funding.

The key message is that computing is changing more rapidly than ever before, and scientists have the unprecedented opportunity to change computing directions. 2004 was a great turning point. At that point, PCs were primarily used in modeling climate change. In 2005, clusters used 12 years of legacy message-passing-interface (MPI) applications as a base.

In September 2004, Intel announced that it would no longer build faster microprocessors. Moore's Law was no longer operating. One could not push up the power anymore. One had to replace speed with parallelism. So multi-core chips were used in PCs and other machines. The economic drivers were no longer there; the architecture and programming models are about to change.

The first petaflop machine was built by IBM for LANL with 1026 Tflop/s on LINPACK reported on June 9, 2008. It had 6,948 dual-core Opteron processors plus 12,960 Cell chips.

The Cray XT5 at ORNL reached 1 Pflop/s in November 2008. The Jaguar, made up of the XT5 and the XT4 has a total of 181,504 cores.

In the top 500 machines, there is only one single-core system: the Earth Simulator (in Japan), which was decommissioned a couple of months ago. 76.6% of the machines have four cores per socket, and 0.2% have 16 cores per socket.

The summed performance of all the top-500 computers has grown linearly from 1994 to 2009, doubling every 11 months. That trend cannot continue. Such a concept is the illusion of continuity. But one has to desire to stay on this curve. An exaflop might be reached by 2020.

Concurrency jumped in 2004. The average parallelism for an exaflop computer will require a million parallel processors. The advance in parallelism will occur at the laptop level, also. As a result, there will be opportunities for new applications.

Moore's Law has been reinterpreted: The number of cores per chip will double every 2 years. Clock speed will not increase and will possibly decrease. Software scientists will need to deal with systems with millions of concurrent threads. And they will need to deal with inter-chip parallelism as well as intra-chip parallelism. A new generation of productivity tools will be needed.

Multi-core comes in a wide variety, such as multiple, parallel general-purpose processors and multiple application-specific processors. The processor is the new transistor. The Intel 4004 had 2312 transistors/chip; there are now thousands of processor cores per die.

What will come next? There is a lot of churn in the system. Some of the architectures seen are all large-core machines, mixed large- and small-core, all small-core, many small cores, many floating-point cores, and 3-D stacked memory.

A likely trajectory is that central processing units (CPUs) will change from multithreading to multicore to many cores, and graphics processing units (GPUs) will evolve from fixed-function to partially programmable to fully programmable. These trends might merge to form the future processor by 2012.

After a period of rapid architectural change, a future processor architecture standard will likely be settled upon. A good bet is that Intel will continue to be a market leader. The impact that this disruptive change will have on software and systems architecture is not yet clear. It might be speculated that the current software will need to be rethought and redesigned, producing a challenge similar to that of the 1990 to 1995 transition to clusters and MPI. Interestingly, the Roadrunner computer has the model of the future with clusters and a complicated node architecture on the socket.

Obviously, MPI will not disappear in 5 years. By 2014, there will be 20 years of legacy software in MPI. New systems will not be sufficiently different to lead to a new programming model.

In addition to MPI, parallel global address space (PGAS) languages, autotuning, compute unified device architecture (CUDA) and Open Computing Language (OpenCL), and/or a wildcard from the commercial space will likely play a role.

Why not MPI everywhere? One MPI process per core is wasteful of intra-chip latency and bandwidth. MPI has weak scaling. And MPI cannot deal well with heterogeneity. It will need to be MPI plus something else.

The likely high-performance computing ecosystem in 2014 will include many-core CPUs and GPUs that are driven by commercial applications and that run MPI plus autotuning, PGAS, or something else in next-generation clusters with many-core or hybrid nodes.

The long-term trends until 2019 were looked at by the Defense Advanced Research Projects Agency (DARPA) Exascale Study, which was commissioned by DARPA to explore the challenges for Exaflop computing. Two models for future performance growth were identified: (1) the simplistic model in which the power for memory grows linearly with the number of chips and the power for interconnect stays constant and (2) the fully scaled model, which is the same as the simplistic except that memory and router power grow with peak flops per chip. The DARPA study's key finding was that the exascale will not be reached with the simplistic or the fully scaled models, and the power costs will be staggering. The power usage must be reduced and capped at 20 MW. There are many other challenges (e.g., in link bandwidth, wires per unidirectional 3-D link, memory bandwidth per node, and power in memory input/output) that would require the development of a lot of technology.

PC technology is no longer an innovative technology. It is no longer performance driven. As a result, PC sales have dropped off as sales of high-definition televisions, DVDs, and other electronic devices have grown. Computer companies are going into other businesses (e.g., iPods).

Why not build a computer out of iPhones? There is a need to use low-power, mass-produced technologies. That is the goal of the Green Flash initiative at LBNL, an alternative route to exascale computing that targets specific machine designs to answer a

scientific question and that uses new technologies whose development is driven by the consumer market.

A challenging application would be cloud simulation. Clouds are important but poorly simulated. The direct simulation of cloud systems must replace statistical parameterization. Cloud models need about 1-km resolution to get transformational change. This increase in resolution is being accomplished by David Randall's icosahedral code, which will require a minimum 20-million-way parallelism. With today's AMD Opteron technology, that would require 179 MW; the IBM BlueGene/P would require 20 MW. The proposed Green Flash technology would require 3 MW.

A design for low power would rely on more concurrency, which would produce a cubic power improvement with a lower clock rate, enabling the use of simpler cores that use less area (and therefore produce lower leakage) and reduce cost, all tailored to a particular application to reduce waste. This is how iPhones and MP3 players are designed to maximize battery life and minimize cost. With small processors, one can come up with a sustained 2.7-Tflop/s computer.

In summary, there are major challenges ahead for extreme computing in terms of power, parallelism, and many other factors not discussed here. Completely new approaches and technologies will be needed to reach the exascale level, opening up a unique opportunity for science applications to lead extreme-scale systems development. There could only be one or two of these systems, so interagency cooperation and a vendor-led partnership will be needed.

Petsko noted that the human-machine interaction is much easier on PCs than with high-performance computers and asked how one overcomes that challenge. Simon replied that that problem has not yet been solved. He knows that the problem exists. There will never be a lack of demand for high-performance computing, so not a lot of attention has been paid to the problem. Data rates are increasing and will outstrip the desktop analysis capabilities. Cloud computing may offer a solution.

A break was declared for lunch at 12:30 p.m.

Tuesday, September 1, 2009 **Afternoon Session**

The meeting was reconvened at 2:00 p.m. **Sharlene Weatherwax** was asked to give an update on the activities of the Biological Systems Science Division (BSSD) of BER.

The BSSD Science Focus Areas (SFAs) include genomic-science fundamental science, the genomic science of biofuels, low-dose radiation, and radiochemistry and instrumentation. In January 2009, program plans from all of the national laboratories were approved. In May 2009, full science-research plans were received and sent out for merit review. In July 2009, there was an external merit review by a 31-member panel for overall scientific and technical merit, appropriateness of the proposed method or approach, competency of the personnel and adequacy of the resources, reasonableness of the budget, management and performance documentation, and suitability of the SFAs for the national laboratories. Summary findings and recommendations were communicated to national laboratory point of contact. The possible classifications were to accept, accept with revisions, revise and resubmit, and reject. The full spectrum of classifications was used. Responses are due on December 24.

Four division solicitations were issued and have closed in the past year: 08-21, Low Dose Radiation Research - Integrated Program Projects, which specifically looked for partnerships; 09-03, Joint USDA–DOE Plant Feedstock Genomics, which added sustainability issues; 09-08, Integrated Radiochemistry Research Projects of Excellence, which focused on new techniques for tracers; and 09-18, Radiochemistry and Instrumentation Research, which provided, inter alia, training for graduate students in radiochemistry (the NIH is interested in cooperating on this solicitation). One division solicitation was issued and has not yet closed: 09-25, Biological Systems Research on the Role of Microbial Communities in Carbon Cycling. In addition, the Knowledgebase solicitation was about to be issued with LOIs due in early November.

The Radiation Effects Research Foundation (RERF) is a bi-national Japan–United States research organization dedicated to the study of health impacts of radiation in survivors of the atomic bombings in Hiroshima and Nagasaki. DOE and its predecessor agencies have funded this effort since 1947; current funding is \$14 million per year. DOE has an interest in understanding the health effects of radiation exposure for the purposes of protecting workers at DOE sites, and BER has responsibility for overseeing the protection of human research subjects in all research conducted at DOE institutions, supported with DOE funds, and conducted by DOE and DOE laboratory personnel; in this role, it is charged to conduct periodic reviews of the human subjects protection programs at DOE labs and other institutions funded by DOE.

BER conducted an onsite review of the RERF’s program for the protection of humans research subjects in July 2009. The Summary of Findings indicates that RERF has an exceptionally high level of commitment to the protection of the rights and welfare of its unique research population and that overall practices meet or sometimes exceed U.S. and DOE human-subject-protection requirements. The key recommendations are to improve the documentation to the level of U.S. requirements, to provide additional training of Institutional Review Board (IRB) members and RERF researchers, and to broaden the representation of the IRB membership.

A workshop was held on New Frontiers in Characterizing Biological Systems. Its scope was the technical capabilities needed to answer the most urgent scientific questions about biological and environmental systems. Participants included experts in all types of imaging technologies and leading researchers in the BER mission areas. The key findings were that technologies are needed to add extra dimensions to biological measurements; to identify important events in heterogeneous environments; to complete the “parts-list” of the cell; and to integrate information for predictive understanding.

Some of the science highlights from the Division are

- The largest simulation model of lignocellulosic biomass deconstruction, which was a SciDAC [Scientific Discovery Through Advanced Computing] project on the Jaguar computer,
- From a call to understand biohydrogen production, an integrated approach to metabolic network analysis and annotation of gene function,
- From the USDA–DOE feedstock genomics program, the identification of an important component of the sorghum lignin biosynthetic pathway,
- New synchrotron technologies enhance the chemical understanding of cellular function,
- New evidence for differences in radiation-induced gene expression, and

- Positron emission tomography (PET) detector development for plant biology.

The three Bioenergy Research Centers (BRCs) are preparing for their second-year onsite progress reviews, which will be held in September and October. An external review team will evaluate their science and management and their progress against stated milestones. Some highlights of the science coming from these centers are

- An improved multiplex expression screen for the discovery of biomass-degrading enzymes,
- Substrate-specific changes in *C. thermocellum* cellulosome composition, and
- Structural characterization of a heat- and acid-tolerant cellulase enzyme.

The JGI had a review in December 2008 that had the key recommendations of improving informatics capabilities, establishing standard operating procedures to facilitate project and data management, and consolidating funding to single point of responsibility. The JGI is a user sequencing facility, and its sequencing targets for 2010 are 20 bacteria and archaea, 8 bacterial resequencings, 2 expressed sequence tags, 15 eukaryotes, 6 eukaryotic resequencings, and 20 metagenomes.

Ahead lie (1) principal investigator meetings in genomic sciences, radiochemistry and imaging instrumentation, and joint USDA–DOE plant feedstock genomics and (2) workshops in supercomputing and plant and animal genomes.

Stacey asked if the genomic sciences workshop will include reports from the BRCs. Weatherwax replied, yes. There will be a genomic science investigator meeting on February 7–10, 2010, in Crystal City.

Wall observed that the three BRCs, when set up, were not encouraged to share information and technology. She asked what steps have been taken to increase such cooperation. Weatherwax replied that such steps had, indeed, been taken. The centers are to provide data in a shared environment and to coordinate meetings among the BRCs. They will have sessions together at workshops and provide joint briefings to the Director of SC.

Stacey asked how DOE is interfacing with NSF's i-Plant. Weatherwax answered that DOE is in discussion with them to ensure that anything they find is able to go into the Knowledgebase.

Joachimiak asked how the BRCs can bring in outsiders. Weatherwax replied that, each year, they sum up accomplishments and draw up new plans. At that point, they can bring new partners on board.

Braam asked how they find out who can contribute. Weatherwax responded that, if they have a need, their researchers are in contact with their communities and can make the center aware of who could contribute.

Sayler asked how big the university research portfolio was. Weatherwax replied that the portfolio was about 40% national laboratory and about 60% university.

Wildung asked how priorities were set. Weatherwax answered that the priorities were set at the division retreat. New people have come into the program with new ideas. Priorities were also set by the participants of workshops. Continued communication is also important.

Michael Kuperberg was asked to provide an update on the activities of the CESD.

The national laboratory SFAs are important to BER. Seven integrated science plans came in from seven national laboratories in May 2009. A merit review was conducted by

15 panelists from a range of disciplines and institutions on July 9-11, 2009. In August, the findings and recommendations were communicated to the national laboratories. Also, the Office set up the triennial review schedule with two national laboratories being reviewed each year. Subsurface Biogeochemistry had two triennial reviews this year (one each for ORNL and ANL).

Three division solicitations were issued and have closed in the past year: 09-15, Climate Modeling: Simulation at Regional Scale (a university solicitation) for which 72 applications were received and 17 were funded for a total of \$6.8 million; 09-06, Climate-Change Modeling (a national laboratory solicitation) for which seven proposals were received and three were funded for a total of \$13 million; and 08-30, Environmental Remediation Sciences Program (a national laboratory solicitation) for which five proposals were received and one was funded for \$1.2 million.

The current solicitations are 9-07, Environmental Remediation Sciences Program, the 107 applications received will be reviewed in October, and 09-16, Climate Change Research in Terrestrial Ecosystems (a national laboratory solicitation) that will look at elevated CO₂ and elevated temperatures in arctic latitudes with above- and belowground heating technologies for which four full proposals were received and will be reviewed and awarded in FY10.

Several planning meetings with BERAC members were held for the Workshop on the Next-Generation Ecosystem Experiment. A series of criteria have been developed that say that this experiment should be in ecosystems that are important globally with respect to potential feedbacks to climate change, in ecosystems that are expected to be sensitive to climate change, with ecosystem-climate change combinations that have been relatively understudied, and with feasible location/technology needs. Four ecosystems fit these criteria: tropical forest, tropical savanna, boreal forest, and arctic tundra (which seems the most feasible in the near term). The Workshop was held in Salt Lake City where exceptional group of tundra ecologists and large-scale ecosystem experimentalists gathered for a full day of input and discussion. The results of the workshop are that

- A warming/elevated CO₂ experiment in arctic tundra would be very important to climate-change research.
- The experiment could be built around the high-level question, what is the overall climate change feedback potential in the arctic?
- It could be very large and involve albedo, CH₄, and CO₂, at least.
- The “active layer” thickness and hydrology would be central.
- The what, how, and when of treatments and measurements will be critical.
- Wide community participation should be facilitated.

The next steps are for BER to issue a technology solicitation, review the proposals, consolidate input, and continue working with the community.

The Division is supporting

- A multigroup effort in modeling extreme events at high resolution to determine how much resolution is needed, where, and why while leveraging DOE capabilities in high-performance computing;
- Carbon cycling in mature forests to see if they are, indeed, carbon neutral as all the models assume (but finding that they are actually carbon sinks);

- Global warming in boreal forests (showing 10-day-earlier bud burst in the spring, greater shoot-length growth, reduced live fine-root biomass, and reduced soil-surface CO₂ efflux);
- Representing cloud-radiation effects in climate models in three dimensions rather than one; and
- Advanced subsurface 3-D transport computing, a case where a simple model is not sufficient.

CESD has two facilities. The first is the ARM Climate Research Facility (ACRF). It received ARRA investments for equipment upgrades that will make ACRF unique and give it the most sophisticated atmospheric radiation measurement capability in the world. So far this year, it has hosted more than 800 users, resulting in more than 185 publications in the scientific literature. The mobile facility is currently deployed in the Portuguese Azores islands; the second mobile facility is under construction for deployment in 2010. The base and underlying programs are working on a strategic planning update. The ACRF has conducted experiments in several climatically important regions at the fixed sites, on Graciosa Island in the Azores, on a mountain top in Chile, and in China. Peer-reviewed experiments have addressed critical science questions including carbon cycling, marine clouds, low-altitude liquid-water clouds, and climatic effects of aerosols.

The other facility is EMSL. It received \$60 million in ARRA investments for recapitalization of aging infrastructure and expansion with new capabilities. So far this year, it has hosted approximately 500 users, resulting in more than 257 publications in the scientific literature (including 11 journal covers). It is implementing new plans and processes from the 2008 review. Recently, it has assembled an international research team, used EMSL surface science and imaging capabilities, used antibody-recognition force microscopy to map the cytochrome locations of two *Shewanella oneidensis* MR-1 surface proteins, and found that MtrC is spread across the cell surface and that OmcA is localized at the cell-mineral interface. This work helps in the understanding of the role of cytochromes in electron exchange with potential application to bioremediation.

Integrated assessment (IA) received ARRA investments for new computers to give more complexity and capabilities to IA models.

Roger Dahlman retired.

Stacey asked if the national laboratories were still resisting the SFAs. Kuperberg replied that the national laboratories do not complain to DOE. One cannot argue against SFAs. The national laboratories are special resources that should be doing specialized research. The SFAs are ways to get them to do those special tasks. Palmisano added that there was some angst about the change, but laboratory leaders saw the benefits of the SFAs. Stacey asked if their effectiveness will be assessed. Kuperberg replied that some subset of the national laboratories will be reviewed each year. Stacey asked about the SFA in general. Palmisano answered that it will probably take a couple of years of experience before BER and BERAC can consider an assessment.

Sayler said that some consider that out-of-the-box thinking is pushed aside by the SFAs, and he asked how those problems got attention. Palmisano replied that innovation is not *encouraged*, but *expected* from the national laboratories. Kuperberg said that the SFAs allow the national laboratories great flexibility in their areas of expertise and give them budget authority to pursue what they choose.

Wildung asked if the SFA awards specified high-risk/high-reward components. Kuperberg said, yes, that was part of the request.

Ehleringer asked if there were any hesitation about the target next-generation ecosystem experiment. Kuperberg said that the hesitancy is about the scale of data and the experiment's size. This experiment is expected to hit the ground in 2012. There will be a minimum set of parameter requirements.

A break was declared at 3:33 p.m. Petsko departed. The meeting was called back into session at 3:45 p.m. **Robert Vallario** was asked to summarize the BER Workshop on Science Challenges and Future Directions in Climate-Change, Integrated-Assessment Research.

The workshop goals were to identify research needs and opportunities for understanding climate-change integrated assessment, to provide an assessment of where the science and technology now stand and where barriers to progress might exist, and to describe potential directions for fundamental research that can be pursued to meet these goals. The specific scope was to explore research ideas and emphases that will help shape the future of the Integrated Assessment Research Program (IARP); to respond to the rapidly changing scientific questions and challenges; to address needs from global and national to regional and local scales and connections; to strengthen the scientific foundations and rigor upon which integrated assessment is based; and to look boldly and comprehensively at the research needs that the nation must address to move forward in mitigation, vulnerability, and adaptation planning.

The workshop was held November 13–14, 2008 in Arlington, Va. It included a general introduction and overview, followed by nine focused technical sessions, and concluding with a wrap-up session and a report out by rapporteurs. The technical sessions were on

- Decision support and the frontiers of integrating systems science
- The grand challenges of impacts, adaptations, and vulnerabilities
- Research needs for mitigation
- Scales: Regional and next-generation sectoral modeling at finer time scales
- Collaborations and interoperable frameworks for the new science challenges
- Transformational science and technology
- Data and data management
- Risk, uncertainty, testing, and diagnostic methods
- New horizons in integrated assessment foundational research

The workshop had 40 participants from academia, industry, and federal agencies.

At the most basic level, the field of integrated assessment is focused on understanding and modeling the complex interactions of human and natural systems; exploring developmental pathways, emissions, the role of energy innovations, and mitigation strategies; providing insights into climate change impacts, adaptations, and the effects of combined, multiple stressors; and developing global, national, and regional perspectives within economic, risk and other policy-relevant frameworks. It does not do policy analyses but delivers toolsets that the planners use. Its models and research were used to produce SAP 2.1.a, *Scenarios of Greenhouse Gas Emissions and Atmospheric Concentrations*.

Working Group 1 dealt with mitigation, transformational science and technology, and complex interactions looking at linkages and dynamics of combined mitigation and adaptation, natural resources and other issues at larger scales, understanding and modeling of the translation of scientific discovery into technology and systems innovation, and use of integrated-assessment models to develop insights into interactions among different components of the human-climate system.

Working Group 2 dealt with impacts, adaptations, and vulnerabilities and looked at 30 species' effects during the next 300 years. The needs of the current models are driven by temporal and spatial resolution and the dynamics of tipping points.

Working Group 3 dealt with spatial and temporal resolution and looked at process scaling and nonlinearities; interfaces among physical, economic, and impact, adaptation, and vulnerability (IAV) model components (e.g., health) in the United States (the process gets worse when one considers the international perspective); data matching to scales; and scale and model uncertainties. It asked whether one would get different answers if one worked from the bottom up rather than from the top down.

Working Group 4 dealt with risk, uncertainty, and diagnostic methods, looking at the modeling of risk and the quantification of different kinds of uncertainty relating to data, parameters, and model structure and at model intercomparisons. Different communities have different perspectives of risk.

Working Group 5 dealt with interoperable and accessible modeling frameworks, which need interoperable input and output detail, time steps, and scales; interdisciplinary modeling environments; agile modeling frameworks for approaching questions of different user communities; community modeling approaches; and multiple models for scientific learning.

Working Group 6 dealt with data development and accessibility, confronting challenges in data quality and verification; data management, distribution, and access; and supporting cyber-infrastructure. Since the workshop, \$4.9 million has been invested in computational infrastructure plus an allocation at NERSC. Clusters at the Massachusetts Institute of Technology currently require 3 weeks for a run for an integrated-assessment model. This community is supercomputer-ready.

The workshop report was completed in June 2009. Printed copies and CDs are available. It has been distributed to participants. Distribution is planned within the USGCRP and other, select communities. The workshop's results are being used for program planning.

Arthur Katz was asked to summarize the BER Workshop on New Frontiers in Characterizing Biological Systems.

The workshop's purpose was to identify new tools and analytical approaches for characterizing cellular and multicellular level functions and processes that are essential for developing solutions for DOE missions in biofuels, carbon cycle, low-dose radiation, and environmental stewardship and to look at a wide range of characterization technologies.

Three questions were formulated for discussion at the workshop:

- What are the biological/environmental processes we need to understand?
- What are the limitations of current technology in addressing these needs?

- What technical capabilities do we need to answer these most urgent scientific questions?

The workshop was held on May 13–14, 2009, in Bethesda, Md. It included plenary presentations on science needs, three parallel breakout sessions, and a report out by the breakout co-chairs. The breakout sessions were based on three scales of processes: cellular processes, which included electron transport and energy production; multicellular processes, which included biofilms, termite gut, microbial communities, and tissue radiation responses; and system-interface processes, which included plant/microbe, microbe/mineral, and molecular-machine materials.

Questions posed to the breakout sessions were

- What are the most significant scientific challenges in your field of research, and what information do you need to make significant advances?
- What are the promising tools and technologies to address these information gaps?
- What approaches or technologies would represent breakthroughs?
- Are there specific questions that require information developed at more than one scale?

The workshop participants reconfigured these questions into four key issues:

1. Adding dimensions to biological measurements. There was a feeling that there were several technologies that, if pressed, could move the boundaries of what can be measured. Currently, one can localize in the microbe target molecular species with high resolution. But that does not give the whole picture. One would like to know the physical location of the target microbe in its biological and abiotic environment and to be able to measure the flux of molecules in and out of the target cell.
2. Identifying important events in heterogeneous environments, measuring and associating rare events or minority components that are difficult to get at and to measure them in as natural (complex) a setting as possible.
3. Completing the “parts-list,” capturing cellular components (e.g., metabolites and carbohydrates) that are currently invisible or poorly characterized, manipulating the activity of these poorly characterized components to understand their functional significance in parallel with their genomic sequencing.
4. Integrating information for predictive understanding, which brings a need for creating tools for the integration and interpretation of complex data sets, developing databases and computational approaches for integrating measurements and models at multiple scales, and constructing iterative feedback systems between experiment and modeling in real time to observe emergent insights.

The workshop steering committee is currently completing the workshop report and executive summary. Substantial written materials produced by the working groups have been organized and integrated. Co-chairs and other participants have had regular telephone conferences to review drafts of sections of the report. A final version of the report is under way. The target date for completion of the final draft is September 30, 2009. The report is expected to be posted by October 15, 2009 on http://www.sc.doe.gov/ober/BER_workshops.html.

Adelstein commented that there are still lessons to be learned. For example, the so-called Warburg Effect in cancer cells showed that cancer cells live by anaerobic glycolysis. If the uptake of fluorodeoxyglucose (FDG) is a surrogate for this complex

system and if it also works in plants, one could define an index molecule that would be useful as a surrogate measure of the complexity of the plant processes. Fowler stated that, in her program, FDG had been fed to a plant and it did, indeed, make FAC cellulose. That makes a good case for having raw metabolic probes for some of these other systems.

Stacey asked if the Committee had any other comments or issues. There being none, he opened the floor to public comment.

Doug Ray (PNNL) noted that there needs to be a balance between the software and the hardware, and continued support needs to be provided for the users to make a community model work.

Wong, staff member, House Committee on Science and Technology, noted that the House Committee on Science and Technology will conduct a full reauthorization of SC next year and is open for input from this Committee.

Stacey complimented the Committee for its engagement and adjourned the meeting for the day at 4:29 p.m.

Wednesday, September 2, 2009 Morning Session

The meeting was called back into session at 9:00 a.m. Palmisano introduced Ari Patrinos, former Director of BER, to the Committee. **Daniel Drell** was asked to introduce Eddy Rubin. Drell pointed out that JGI had undergone a triennial review in December of 2008. That review made a series of recommendations: In science, JGI was asked to clarify its relationship with PNNL, to describe its investments in sequencing phases, and to cross-fertilize different sequencing programs. In operations, it was asked to cross-partner the laboratory information management system, to monitor the Community Sequencing Program for reviewer diversity, to implement more-frequent microbial proposal reviews, to link the annual survey to the user meeting, and to continue its commitment to safety and health. In informatics, it was asked to fix deficiencies in informatics leadership, to find and hire a world-class Chief Information Officer, to implement an immediate-release-of-of-raw-reads data policy for non-BRC projects, to design JGI informatics tools for maximum interoperability, and to reconsider idea of JGI as an “analysis only” center. In management, it was asked to centralize management and funding through LBNL (as the prime contractor), to ensure that the JGI Director has the clear authority to configure all JGI efforts, and to engage a Chief Technology/Information Officer.

Implementation of these recommendations has proceeded. In February 2009, there were calls from BER to JGI-partner national laboratory directors and to assistant-laboratory-director managers. Since then, there have been biweekly partner calls. The Joint Management Board (now the Joint Coordinating Committee) met in March and August 2009. Between October 2009 and the end of FY10, JGI funding will be centralized through LBNL (except Hudson-Alpha for FY10 only). Complete centralization of funding will be in effect in FY11. In August of 2010, there is going to be an informatics review.

Eddy Rubin (1) summarized the 2008 BER science and operations review, which was conducted on Dec 3-5, 2008, and reported on March 3, 2009, and (2) reviewed the JGI 5-year strategic plan.

In 2009 to date, JGI has produced 81 peer-reviewed publications and its publications have been cited 18,919 times in the literature. Major publications this year were the sorghum genome and two algal genomes. Upcoming major publications are the Genomic Encyclopedia of Bacteria and Archea, the brachypodium genome, and the soybean genome.

The review's clear message was to establish a centralized management and an organizational structure and to establish a funding flow from LBNL to partners to align authority and responsibility. The structure that the reviewers saw resulted from there being three DOE genome centers that contributed to different programs. The new structure is much more straightforward with coordinated funding and programs that set their own research agendas. Activities are still distributed among Walnut Creek, LANL, and ORNL. Guidance and oversight are provided by BER and the Director of LBNL with input from the Science Advisory Board, the Joint Coordinating Committee, and the User Committee.

A JGI science program management model has been implemented, science program leads have been named and are functioning, and program-based financial planning and reporting has been implemented. The model is in place and is working.

In informatics, senior leadership deficiencies needed to be remedied because of concern about the informatic planning and hardware infrastructure, which faces dramatic increases (by a factor of 1000 in a few years) in data generation. The next generation of technology needs to be planned for. This issue is taken very seriously. An Informatics Department Head has been hired: Svilen Tzonev. The new position of JGI Chief Informatic Officer has been created and will be filled; currently, Jill Mesirov is consulting in that role. Another new position, JGI Informatics Project Management Program Head, has been filled by Evi Dube. A new Informatics Advisory Committee will have its first meeting in December 2009. \$11.1 million in ARRA Funding Targeted for IT upgrades to add infrastructure for management, storage, and movement of genome-scale datasets. storage will increase 100%, JGI's central computing cluster will be upgraded by 200%, and ESnet access will be upgraded. Funding for these changes was received on August 7. JGI is exploring the national laboratories' high-performance computing capabilities to help JGI's data challenges. Projects are already under way at PNNL, LBNL, ANL, and LLNL.

There were 23 review-committee recommendations, 10 in informatics, 7 in operations and safety, 4 in science, and 2 in management. JGI has implemented or is implementing all the recommendations and is keeping Gantt charts on its responses. A *JGI 5-Year Strategic Plan* is being prepared.

Sequencing technology is being driven by the desire to be able to produce an individual human's genome. A 30-fold increase in sequencing has been seen in a very small period of time. JGI's mission in going forward is as a user facility for large-scale genomics and analysis to enable bioenergy and environmental research with unique capabilities in carrying out genomics of sufficient focus, scale, and complexity to help users solve important but hard DOE-relevant problems.

The *JGI 5-Year Strategic Plan* is broken into plants, microbes, metagenomes, and the user facility.

In plants, there is a roadmap: the National Research Council's plant genome report of 2008, which said, "It is critical that JGI continue to serve a broad remit for sequencing and resequencing of plant genomes" Priority lists of genomes to be sequenced are compiled by the research community. JGI has limited resources, so some of these genomes will get flagship treatment (high-quality and -accuracy), and some will get less-intensive attention. The problem with plant genomes is that, although one might have the sequence, one cannot assign function to most of it. We might have the book, but we cannot read it. One way to determine function is to sequence several similar genomes and analyze the genomic differences. For example, JGI will sequence and analyze 12 *Arabidopsis* relatives to identify functional elements in these genomes based on evolutionary constraint and to provide a roadmap for similar projects in plant groups with much larger genomes. The goal of the JGI plant program is to produce the genomic tools necessary to understand cell-wall construction, feedstock production, and carbon sequestration and sunlight-energy-harvesting pathways. All of JGI's projects will feed into this goal.

In microbes, JGI is the major sequencer of genomes, producing about 30% of the world's complete archaeal and bacterial genomes. Three-quarters of all sequenced genomes belong to just three bacterial phyla. This limits the linking of one genome to similar ones to identify genes and to determine their functions. One would like to have stepping stones from one genome to another to another. Therefore, JGI has started compiling a pilot Genomic Encyclopedia of Bacteria and Archaea (GEBA) with the sequencing and analysis of 64 genomes. The final stages of this work are with *Nature* for review. The reviewers have been quite laudatory, and the included genomes are relevant to DOE. An analysis of *H. Utahensis*, which grows in the Great Salt Lake with a salt concentration 6 times greater than that of the oceans, revealed a cellulose gene cluster that has applications using ionic liquid detergents for cellulose dissolution. A DOE Bioenergy Center has subsequently synthesized *H. Utahensis* cellulases to use their high-salt cellulose activities. The ultimate goal of JGI's microbial program is to reveal bacterial and archaeal diversity, including major uncultured phyla, which will require technologies for accessing the genomes of hard-to-culture organisms. These presequencing technologies will be made available to extramural users.

In fungi, the major genome projects worldwide are at the Broad Institute, JGI, and Washington University. JGI is going to focus on fungi in four categories, those involved in plant feedstock health, lignocellulose degradation, fermentation, and industrial applications.

JGI metagenomic projects include the digestive processes of cows, dung beetles, shipworms, a bird that digests leaves, and kangaroos. Metagenomic plans are guided by the National Research Council's report, *The New Science of Metagenomics*, which recommended the establishment of a small number of large-scale projects to study particular habitats. Soil represents a habitat that is important due to its role in carbon and nitrogen cycling and biomass production. It is a particularly "gnomically" challenging environment because of its complexity. The Great Prairie Soil Metagenome Project will look at Iowa never-tilled prairie and Iowa land tilled for corn for more than 100 years because the Midwest prairie represents the largest expanse of the world's most fertile

soils, it sequesters the most carbon of any soil system in the United States, and it produces large amounts of biomass annually, which is key for biofuels and carbon sequestration. The information from this project will be used to improve soil management, improve carbon sequestration, and potentially manage traits such as greenhouse-gas fluxes and carbon stability.

The termite hindgut study produced 62 million base pairs (Mbp). The Great Prairie Soil Metagenome Project will produce 1000 times as many, and the Grand Challenge Project will likely be a terabase project. Potential foci for the 1-Tb Grand Challenge Project include sequencing the 12 major soil types to cover the extremes in soil diversity (e.g., permafrost to tropical desert to alkali flats to taiga forest to wetlands) to discover gene adaptation to environmental extremes.

Looking forward, the JGI is considering potential emphases on analysis, providing chromatin-immunoprecipitation (ChIP) sequencing, resequencing, genomic capturing, transcriptomics, mapping, and single-cell genomics. It can isolate full-length lignocellulosic genes and produce a number of full genomes, but the analysis of 18 GB of data would take about 70 CPU years on a PC and about 3 weeks on JGI's 1500-CPU cluster. The projects embarked upon now face a computational bottleneck. JGI needs to partner with the high-performance-computing community. Therefore, it is sponsoring a workshop on high-performance computing for next-generation sequencing with a focus on bringing national-laboratory computational infrastructure and expertise to bear on problems associated with the volume and nature of the next-generation sequencer's output.

Stacey noted that there are other functional elements besides genomes and other processes and asked how JGI views these other components. Rubin replied that JGI can contribute to all of those elements and link that information to the Knowledgebase. The genome centers can do the sequencing portion that is their unique capability and that is available to a wide variety of research programs.

Braam agreed that the idea that one can grab onto genomes that are related to learn gene function for diverse organisms makes a lot of sense. But at a deeper level, the organisms are different in part because the genes and the organism's functions have diverged. So, part of the assumption that one makes about the groups being similar makes it difficult to answer the question of how one can get to see any difference. Rubin replied that the closer one got to a nearest neighbor, the better one can call a gene. It works quantitatively at some level. These are hard problems.

Riley noted that the JGI is doing hypothesis-driven research. Rubin agreed and said that that is why GEBA is needed, to provide a reference genome.

Ehleringer noted that there is a huge difference in productivity between the C3 and C4 taxa and asked if any consideration had been given to the comparative genomes of these taxa. Rubin replied, essentially, no.

Remington asked how one can leverage the different capabilities of all these different JGI functions. Rubin replied that, within the plant program is an assembly group; then the informatics group moves information around. Because each program has its own information group, one has to make sure that the managers talk to each other. Remington said that she was thinking more about scientific opportunities. Rubin answered that there is no distinction between microbial and plant programs. The JGI has a single group that guides the whole effort. Remington asked if there were any mechanism in the Strategic

Plan to do this. Rubin responded that the JGI is looking for synergy, and the users are great drivers of scientific direction. They pushed the JGI to have different groups to work together and to use techniques for different purposes.

Sayler asked if JGI saw itself providing assistance in pre-sequencing in whole-metagenome analysis. Rubin answered that, in the past, JGI had DNA and a lot of sequences. In the future, it will have a lot of techniques for purifying that DNA, allowing the analysis of microbial assemblages.

Riley asked where the computational effort was going. Rubin replied that JGI cannot deal with a terabase of data. It has concrete problems with the masses of data and cannot deal with those problems. It is reaching out for algorithms and large machines to solve these problems. Riley asked if it were looking for DOE to supply the expertise. Rubin responded, yes; JGI needs to connect with partners, not to generate the capability itself.

A break was declared at 10:09 a.m. The meeting was called back into session at 10:24 a.m. Stacey said that the Committee is expecting a charge letter asking for a BER strategic plan with a 20-year planning horizon. The charge is expected to ask: “What are the greatest scientific challenges in systems science that BER should address in the long term (20 year horizon)? How should we position BER to address those challenges? For example, what continued or new fields of BER-relevant science will the Department need to achieve its future mission challenges? What future scientific and technical advances and workforce developments are needed to underpin BER’s complex systems science?”

A subcommittee has been assembled. That subcommittee has drawn up a tentative plan and schedule to

- Focus initially on the planning and hosting of an overview, strategic planning workshop to be held in Spring 2010
- Identify specific topical areas based on relevance to the BER mission and future promise to direct and focus the discussion at the initial workshop
- Develop subcommittees around each of these topic areas to write initial, short white papers, to identify speakers for the initial workshop, and to participate in the workshop
- Host the workshop from which a planning document will be written to guide the future BER strategic planning efforts.

The four tentative topical areas identified are

- Climate change, for which a 20-year vision for climate change science within BER should include new scales of data collection driven by technological breakthroughs; harnessing computational breakthroughs for regional, global, and extreme-event modeling; identifying and predicting climate-change impacts on resources; and evaluating and optimizing implemented and planned remediation strategies.
- Systems biology, for which the new view strives to move beyond the traditional use of the scientific method to conduct “reductionist” science toward the goal of using modern tools to discover new emergent properties that can only be seen by a systemic view of the entirety of the biological process.
- Information and synthetic biology systems integration framework, for which eavesdropping (through understanding of cell–cell signaling, quorum sensing, allelopathy, symbioses, and host–pathogen interactions) on the flow of genetic

and chemical information across significant spatial and temporal scales of ecological processes will allow altering those pathways to meet sustainability challenges.

- Research framework for energy sustainability, for which drivers like climate and land-use change; food, water, and energy security; and life-cycle assessment in industrial production and agriculture will intersect, requiring research to define, quantify, and ameliorate changes or loss of reliance in the underlying fabric supporting sustainability.

The Subcommittee needs all of BERAC's help to make this strategic planning initiative valuable, relevant, comprehensive, rigorous, and effective. Specifically, the Committee could address the questions: Are the four topic areas identified by the current planning committee the most appropriate? Is the plan for the strategic planning process and the initial workshop appropriate and effective? How does one look 20 years into the future? Who are the other people that should be enlisted in this strategic planning process? And what other questions should be addressed?

Wildung pointed out that these topical areas do not reflect some of the current strengths of BER and asked if those traditional and current capabilities had been mapped onto these topics so that the workshop can build on them. Stacey replied, in general, it is desirable to start with the baseline interests of BER, which is the home of nonmedical biology in the U.S. Government. Randall added that DOE has great strengths that are not mentioned here but will be considered by the Subcommittee, which will add expertise in those areas.

Fowler stated that the workforce for solving these problems has to be built and trained to carry the enterprise through the next 20 years. Wall said that she did not see an effort to build an expertise and capability in informatics. Stacey agreed that informatics and computational biology will be critical in the next 20 years. Remington asked what DOE had to tackle in the next 15 years, pointing out that each group has to fit informatics into its discussions.

Sayler pointed out that there are redundancies across these topics, and Joachimiak asked what the environment was. Stacey replied that systems biology scales from the cell to the ecosystem.

Kingsbury stated that the sustainability topic is a diversion from what BER has done in the past. In addition, one cannot divorce the work being done from policy issues. The sustainability issue might lead to a slippery slope for BER. Reilly added that the Committee will need to know what the boundaries are, and the Subcommittee will need help from the Committee to make those decisions. Palmisano pointed out that there was a joint DOE-USDA meeting last fall on that topic that would be a good model. Kingsbury said that one needs to draw some bright lines

Ehleringer said that the Committee also needs to consider the social sciences and that social scientists need to be on the steering committee from the start. Riley stated that the preliminary list has some social scientists on it and that she would send that list to the BERAC members for suggestions and advice.

Wildung said that a strategic plan implies that one is going to lay out actions for the next 20 years to get to these themes. Palmisano responded that BER is going to follow the example of BES's grand-challenge workshops, in which general topics were first addressed and then a series of focused workshops were held. Under Secretary Koonin

asked for a long-term vision for BER and is interested in attending these workshops. Stacey added that the drafters of the charge letter tried to not be so vague as to be incomprehensible and not be so detailed as to limit discussion.

Penner said that some effort should be made to see how these areas inform each other (e.g., genomics informing carbon sequestration). Stacey replied that there may be some crosscutting themes identified and explored. It might be good for each member to think about and share what they see happening in their own fields during the next 20 years.

Sayler asked how many days the workshop might run and whether there would be a keynote speaker in each topic. Stacey replied that his view was to have a few keynote speakers to be visionary and to challenge the participants, with a consensus developing over two days. A professional facilitator may be used.

Braam said that the white papers might state where the disciplines are now and the strengths of BER, with visionary ideas being brought in with the keynoters. A powerful brainstorming workshop is wanted. She asked Stacey what he saw the purpose of the white papers to be. Stacey replied: to get people to start producing ideas that they then bring to the workshop. Sayler said that he did not expect that the level of participants who are being considered would be interested in background papers. They should be looking deep into the future, not looking to the past. Stacey said that the meeting could be planned to have both. All of this is in the planning stage.

Ehleringer said that there are a number of wonderful programs that DOE already has. Considering their interaction is one way to consider the future of DOE. Stacey added that one needs to make sure that the different subgroups report to each other. He asked the Committee members what they thought the future will look like. There were no responses.

Riley asked if alternative views could be represented. (That is, is there a *better* way to go forward?)

Sayler pointed out that this is not an effort to form an evolutionary path. The first workshop should determine what technology and techniques are coming from other areas during the next 20 years. A leap forward needs to be taken, and those technologies and techniques need to be embraced (e.g., today's out-of-the-box thinking that is going to be the norm 10 or 20 years from now). New ways of thinking about the problems that biological and environmental sciences face need to be considered.

Adelstein said that this initiative has the categorical imperative; it has brainstorming and it mines BERAC expertise. There is a lot of visionary work in the past. The BER facilities serve a very important role. The goodness should not be ignored in planning.

Stacey stated that strengths and opportunities can be identified, trends can be seen, and those trends can be extrapolated out 20 years.

Kingsbury worried that the workshop will introduce redundancy by separating these topics. It needs to identify the barriers that will be faced rather than to plan a pathway. He would break it into three parts, merging into one topic the systems biology and the informatics.

Joachim said that the workshop should be proactive about the future challenges (e.g., going from the microscale to the macroscale to the megascale) instead of being reactive.

Wooley pointed out that the planning that went into the GTL was exceptional and resulted in JGI and other high-quality outcomes. But other agencies did not pick up on it.

It might be good to have the NAS do the study and then have BERAC do an inclusive study. That might carry more clout. Palmisano pointed out that a successful model is being followed, and Brinkman and Dehmer would like to see BERAC ownership of this study.

Ehleringer believed that the Committee should focus on challenges and questions rather than topics. It might be clearer to rephrase these topics as questions and challenges. Sayler asked whether that would be the province of the first workshop. Ehleringer said that he believed that it would focus the attention of the participants and allow of the coupling of ideas.

Wildung said that the workshop needs to identify the key problems that the biological and environmental sciences will face during the next 20 years and then consider how to address those problems scientifically. The Committee might want to consider energy requirements with population growth and identify the key problems, making the science more apparent and leading to a strategic plan.

Bierly stated that the crosscutting problems (education, computing, etc.) have to be solved, and the umbrella is the environment. There are users of this information out there, and the Committee should be asking them where the field should be going. Sayler suggested that maybe the sustainability component could be the organizing principle.

Stacey said that this discussion shows what an enormous task the Committee faces. The Subcommittee will continue to meet by teleconference, and all Committee members are welcome to join in those discussions.

Stacey went on to discuss the new charge. The Committee has been charged to put together a COV to the Climate and Environmental Sciences Division and to examine processes involved in soliciting and reviewing proposals and in making awards. Riley added that the charge also covers how the managers are doing their jobs. Participants on such a COV learn a lot about the real needs. Stacey pointed out that there should be some Committee members on such a COV.

Thomassen pointed out that BER has a webpage of prior COVs and the Office's responses to the recommendations of those COVs.

Stacey opened the floor for new business and comments. Ehleringer suggested getting a progress report on the status of the next-generation global-change experiment and the free-air carbon enrichment (FACE) transition at a future meeting.

Bierly suggested requesting some presentations from other agencies that have huge climate-change programs, like NOAA and NASA.

The floor was opened to public comment. Doug Ray (PNNL) said that the BER program on subsurface science is currently well supported by society and should be considered by the workshop.

There being no further comments, the meeting was adjourned at 11:39 a.m.

Respectfully submitted,
Frederick M. O'Hara, Jr.
Recording secretary
September 21, 2009