Minutes for the
Basic Energy Sciences Advisory Committee Meeting
December 6-7, 2004
Marriott Washingtonian Hotel, Gaithersburg, Md.

BESAC members present:

Nora Berrah
Philip Bucksbaum
Sue Clarke
Peter Cummings
Mostafa El-Sayed
George Flynn
Laura Greene
Bruce Gates
John Hemminger, Chairman
Eric Isaacs
Anthony Johnson
Kate Kirby (Tuesday only)
Walter Kohn
Gabrielle Long
William McCurdy, Jr.
Daniel Morse
Kathleen Taylor
Ward Plummer
Samuel Stupp
Stanley Williams
Mary Wirth

BESAC members absent:

Martin Moskovits
John Richards
Richard Smalley

Also participating:

Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Helen Farrell, Idaho National Engineering and Environmental Laboratory
Bruce Harmon, Deputy Director, Ames Laboratory
Patrick Looney, Assistant Director, Office of Science and Technology Policy, EOP
Michael Lubell, Director of Public Affairs, American Physical Society
Pedro Montano, Office of Basic Energy Sciences, USDOE
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Raymond Orbach, Director, Office of Science, USDOE
Douglas Ray, Director, Chemical Sciences Division, Pacific Northwest National Laboratory
Leslie Shapard, Oak Ridge Institute for Science and Education
Walter Stevens, Office of Basic Energy Sciences, USDOE
Karen Talamini, Office of Basic Energy Sciences, USDOE

About 130 others were in attendance in the course of the two-day meeting.

Monday, December 6, 2004
Morning Session

John Hemminger, Chair, called the meeting to order at 8:56 a.m. and introduced **Leslie Shapard**, who made scheduling, safety, and convenience announcements. Hemminger asked the Committee to read the preliminary report of the Subcommittee on

Theory and Computation during the day and evening; it would be discussed the following day. He asked the members of the Committee to introduce themselves. After they had done so, he introduced **Patricia Dehmer** to review the current activities at the Office of Basic Energy Sciences (BES).

That news was mostly about the budget because, for the past several years, the budget process has not been normal. Budgeting requires negotiating hurdles; each agency and division is competing with many others and is doing so for two fiscal years at once.

The first big hurdle occurs inside the Office of Science (SC). Each associate directorship (AD) determines program priorities within constraints of the funding guidance provided by the Director of SC. Each AD presents program priorities to the Director of SC. Then the Director of SC determines program priorities within constraints of the funding guidance provided by the Department of Energy (DOE). The Director of SC wants to know what the advisory committees think (e.g., as in the 20-year study).

The next hurdle is inside DOE. The Director of SC and the DOE assistant secretaries present their program priorities to DOE. The Department determines overall agency priorities at that point. SC prepares its requests for inclusion in the President's budget. Each SC AD is responsible for the preparation of the AD-ship budget.

At the Office of Management and Budget (OMB), each AD defends the program budget at a hearing in early September. OMB provides "passback" guidance to DOE in late November. Discussions between DOE and OMB refine final budget numbers. And then SC prepares its contribution to the President's budget. Each SC AD is responsible for the preparation of the AD-ship budget. Often, advisory committees produce documents during the summer that support or do not support initiatives (e.g., the hydrogen initiative).

The President's request goes to Congress in February. From March through September, agencies present their budgets to Congress in formal hearings. Advisory committee reports are referred to in these hearings. Congress appropriates funding for 13 appropriations bills for the fiscal year, using the President's budget as a starting point for the congressional budget and appropriations. Congress then does what it wants to do.

Three years of budgets are under way at any time. Currently, the FY05 Omnibus Bill is being passed, the FY06 OMB passback for congressional budget preparation is being received, and initiatives for FY07 are being formulated during December.

In 2003, preparation began on the FY05 budget, proceeding normally and largely on schedule. In 2004, the FY05 President's budget was presented to Congress with funding for research programs about equal to that in FY04, funding for facility operations that was increased modestly, the Spallation Neutron Source (SNS) construction project fully funded, all five nanoscale science research centers' construction projects fully funded, the Linac Coherent Light Source(LCLS) project's funding for engineering design and long-lead procurement, and BES's participation in the President's hydrogen fuel initiative with $21.5 million in new funding for basic research and support of the hydrogen economy. During the summer, there were gloom-and-doom predictions for the FY05 budget because of the large deficit; significant national priorities; and commitments to Medicare, health care, and Social Security. In October, there was no appropriations; that was not unusual. In the past 15 years, only five Energy and Water Development bills have been signed prior to October 1. In the past 5 years, none has been.

In early November, the American Institute of Physics noted that "the fiscal year 2005 Energy and Water Development Bill is even more troubled. Sen. Pete Domenici's (R-NM) subcommittee has not even released a Bill. Funding for the Yucca Mountain nuclear waste repository is a major hurdle. The Bush administration requested $180 million, far more than the $131 million in the House-passed bill. Domenici supports taking $749 million every year from a federal trust that has been funded by the nuclear industry, as well as imposing an additional $446 million from the nuclear utilities as a one-time surcharge. In addition, the House bill and the presumptive Domenici Bill are going to be at loggerheads about the funding of the administration's nuclear weapons initiatives."

DOE plans for a year-long continuing resolution (CR). Under a year-long CR, no new starts would be permitted, which would stop the LCLS long-lead procurement, the Brookhaven National Laboratory (BNL) nanocenter construction, and funding for basic research and support of the hydrogen economy.

In late November, SC received a significant increase in HR 4818, the omnibus appropriations bill. Until the text of this bill was released, it was impossible to determine the parameters of the FY05 budget because only the House had passed its version of the Energy and Water Development appropriations bill. (The Senate bill was never considered by Sen. Domenici's subcommittee.)

The overall budgets for science are mixed. The omnibus bill increases the SC budget $200 million from the FY05 President's request, of which $80 million is congressional direction. Of that, more than $50 million is provided to BES compared with the President's request. The omnibus bill cut the National Science Foundation (NSF) budget for FY05 by about 2%. Funding for the laboratories of the National Institute of Standards and Technology was increased significantly from FY04.

The Committee recommendation for BES is $1,076,530,000, an increase of $13,000,000 over the budget request. For purposes of reprogramming during FY05, the Department may allocate funding among all operating accounts within BES. The conference agreement includes $1,113,530,000 for BES.

BES is going to assume that (1) the $50 million is nonrecurring funding (i.e., it will not appear in the FY06 President's request to Congress), and (2) out-year budgets will be constrained. Therefore, it will allocate the $50 million in a way that minimizes out-year mortgages and addresses critical needs that might not be met with constrained out-year budgets.

The 0.8% rescission to BES and SBIR/STTR [Small Business Innovative Research/Small Business Technology Transfer Program] on the new $50 million account for about $10 million, leaving $40 million to allocate. The remainder will be used for activities such as

- Forward funding of university grants, both new applications and renewals
- Postdoctoral positions
- New-investigator startup funding
- One-time capital-equipment supplements at the national laboratories and universities
- Critical maintenance and upgrades at facilities (e.g., maintenance and fuel at High-Flux Isotope Reactor (HFIR), top-off mode at the Advanced Light Source (ALS), beamline and optics upgrades at the Stanford Synchrotron Radiation

Laboratory (SSRL) to take advantage of increased brightness from the SPEAR3 upgrade at the Stanford Positron Electron Asymmetric Ring, and other high-priority needs at light sources)

- R&D for instrumentation in ultrafast science and for other facility-related activities
- New starts and the incurring of mortgages in priority areas like ultrafast science and theory and computing

No funding has been allocated yet. BES will provide a more complete report at a BESAC meeting toward the end of FY05.

BES's funding is included in the nondefense R&D funding portion of the $2.4 trillion dollar FY05 budget. The American Association for the Advancement of Science (AAAS) produces a very thoughtful analysis of the out-year projections in the annual budget. This year they commented: "President Bush released his fiscal year (FY) 2005 budget proposal in February. The focus of the budget continues to be record-breaking projections of budget deficits; with a deficit of about $500 billion expected this year, a major focus of the budget is the Administration's promise to halve the deficit within five years. In order to do so, the President proposes to keep domestic discretionary spending growth well below the expected rate of inflation while continuing to lavish resources on defense and homeland security discretionary programs, proposing $1.1 trillion in tax cuts over the next decade."

The out-year projections of the AAAS analysis show nondefense discretionary spending declining slightly for the next 5 years. This is not good news. That analysis indicates that the percent change from FY04 funding will be –7% by FY09, and this is an optimistic projection because a 2% deflator was used rather than a more realistic 5% deflator. Real spending power will decrease.

BES was made part (~13%) of the Hydrogen Fuel Initiative with FY05 funding of $29 million. With that funding, two solicitations [one for universities and one for federally funded research and development centers (FFRDCs)] were issued in April 2004. FFRDCs were limited to six submissions as leading institution. There was no limit on the number of submissions for universities. By July 15, 2004, 668 qualified preproposals were received in five categories (which came from the BES workshop). National laboratories were limited to six submissions per laboratory, which equals about 75 submissions. Universities submitted about 600 submissions.

Each preproposal was reviewed by at least one of five panels corresponding to the five submission categories. Each panel consisted of DOE federal officials knowledgeable in the research areas and with responsibilities for managing projects within the Hydrogen Fuel Initiative. The review panels judged the suitability of the preproposals in accordance with DOE's scientific, technical, and strategic goals related to the Hydrogen Fuel Initiative.

Of the 668 preproposals, 261 were selected. The principal investigators (PIs) were notified by September 1, 2004, and full proposals will be due by January 4, 2005. Selected were 215 university preapplications (101 universities in 36 states and Puerto Rico) and 46 FFRDC preproposals (13 DOE national laboratories in 10 states).

The average number of PIs per preproposal was 2.9 for universities and 6.5 national laboratories. The average funding requested per preproposal was $294,700 for

universities and $834,500 for national laboratories. The timeline for the proposal procedure is

January 4, 2005	Full proposals due
February – April, 2005	Proposal Peer Review
April – May, 2005	DOE assesses review and selects awards
June – July 2005	Awards made, pending appropriations

It is anticipated that up to $12 million annually will be available for multiple awards in each of the two main research sectors, universities and FFRDCs.

BES is coordinating with the Office of Energy Efficiency and Renewable Energy (EERE) in the hydrogen storage/hydrogen production solicitations. BES staff (1) provided recommendations on scientific scope of the Grand Challenge solicitations; (2) assisted in developing the external peer review panels of experts; and (3) served as federal reviewers on the award-selection panels.

For the BES basic research solicitation, DOE technology program offices reviewed research topical areas, staff from technology offices were part of the preproposal review process, and SC-1 and the National Hydrogen Program Manager were informed of the award selections. The annual BES Hydrogen Program Contractors' Meeting will be collocated with the DOE Hydrogen Program Review to produce basic–applied R&D crosstalk. EERE, SC, Fossil Energy, and Nuclear Energy Research coordinate on the formulation of program management and operations plans.

Hydrogen symposia are being held at the American Physical Society March Meeting, the American Chemical Society National Meeting, and the Materials Research Society Fall Meeting. An MIT minicourse on hydrogen research is being conducted by Mildred Dresselhaus. *Physics Today* and *IUMRS Facets* are running articles on basic research needs for a hydrogen economy by Crabtree, Dresselhaus, and Buchanan.

A BESAC committee of visitors (COV) reviewed the brand new Division of Scientific User Facilities (DSUF). That committee made 19 specific recommendations, and BES has officially responded to each of them. BES has become more proactive in dealing with issues brought up by such committees. A number of the recommendations by this COV were directed to facility managers, and those recommendations are being addressed in meetings with laboratory directors. The recommendations and the responses to each of them will be posted on the BES web site. The formal report from the COV has been submitted to John Hemminger.

BES is facing some big challenges. It has a number of construction projects under way. It needs to execute well all of its ongoing projects/initiatives and to transition them to robust operation [SNS, LCLS, Transmission Electron Achromatic Microscope (TEAM), five nanocenters, and basic research in support of a hydrogen economy]. It also needs to make SC and especially BES synonymous with energy research. BES wants to increase the understanding of the magnitude of the problem facing society, gain support for a plan of action, and lead in executing the plan. Ideally, the forthcoming solar workshop will help define the bones of that plan. BES also wants to define the grand challenges in BES research for use as a communications and strategic planning tool. Ideally, a forthcoming BESAC workshop will start the process.

BES has always advanced the next generation of tools. One task is to integrate more effectively its activities in the universities and the national laboratories. It has made great steps in that direction in the past few years. A big challenge for all of science is to

manage the impacts of large-scale science. Billion-dollar initiatives gobble up large portions of the budget and must be managed effectively.

Plummer asked who coordinated the Hydrogen Initiative at BES. Dehmer replied, Harriet Kung.

Walter Kohn noted that there is concern about how independent science advice is incorporated into this administration's policy and asked if the scientific community was involved in the runup of the National Aeronautics and Space Administration (NASA) budget or in the identification of the Hydrogen Initiative. He called attention to David Baltimore's piece in the *Los Angeles Times*, "When Science education leaves the U.S." The United States is rapidly slipping in science literacy. Lack of federal leadership is cited as one cause. Kohn said that his sense was that the national laboratories are hurting badly. Dehmer responded that, speaking for BESAC, advisory committees make a big impact. With the hydrogen economy, the Administration got advice from a wide variety of sources, including BES's workshops. On a broad scale, the Administration has had science advice and has responded to and relied on that advice.

Hemminger introduce **Ray Orbach** to speak on the status of the Office of Science (SC). Orbach assured the Committee that its advice on budget priorities comes through loud and clear and that the advice and support of this Committee and community have made the support of SC initiatives very effective. BESAC's reports resonate throughout the government and country. The President, Congress, and others listen to BESAC's advice on such topics as the hydrogen economy, fusion energy, and others. As a result, BES has done very well in the budget process, and SC has done well, also.

A graph of SC appropriations from 1992 to 2005 reflected that success. In 1995, those appropriations declined severely because of the death of the super conducting supercollider. Because of the lack of that facility, CERN will be the center of discovery in future years. Such large-scale facilities can be the key to world leadership in science, and they can't eat up all your resources. The budget is marked by trade-offs between R&D and facilities. You need facilities to do R&D, but they can eat your lunch. The increase in funding since 2000, however, has been impressive. The United States has the leadership of world's science, but if it is not careful, it will lose that leadership. When the upgrade of the SNS is complete, it will have leadership in neutron science for a decade. The LCLS will be able to look at chemical reactions on a timescale on the formation of the chemical bond. This is a decade ahead of the Deutsches Elektronen-Synchrotron (DESY) machine in Germany. This scientific leadership and these facilities have a major influence on world leadership. The Department builds the best facilities and operates them in the best way.

BESAC's advice was critical in the formation of the 20-year facilities outlook plan. It presents a prioritized list, which is not set in stone, of facilities needed by the scientific community. It is divided into three epochs: the near term, midterm, and far term. The SC strategic plan tracks the 20-year facilities outlook. The top six near-term facilities are currently in play.

For the International Thermonuclear Experimental Reactor (ITER), negotiations are ongoing regarding siting as well as legal and financial issues. Dealing with the international community has been an eye opener. What something "costs" is vastly different in the United States, Germany, and Japan. Site selection is under intense negotiations; 28 other issues remain to be addressed (e.g., intellectual property).

For an UltraScale Scientific Computing Capability, the Oak Ridge National Laboratory/Argonne National Laboratory (ORNL/ANL) team is developing a "Leadership Class" machine. The new budget has $30 million more than was in the President's request; $75 million will go into the 75-teraflop machine.

The Joint Dark Energy Mission is one of the most important scientific opportunities in science today. Dark energy accounts for more than 70 percent of the energy budget of the universe. An instrument will be selected in peer-reviewed competition sponsored by NASA and DOE. R&D continues on Space Nuclear Auxiliary Power (SNAP) to look at type 1A supernovae.

Both R&D and conceptual design are under way for the LCLS as well as funding for long-lead procurement in the FY05 budget. Support in the administration and Congress is absolutely solid. There will be lots of surprises discovered by this facility.

R&D is also under way for the Protein Production and Tags Facility, which is part of GTL1 [Genome to Life]. Project engineering and design funding are included in the FY05 budget. This facility is a very interesting example of the interplay between the administration and Congress. Its purpose is to give the full set of tagged proteins to understand cell functions. SC will introduce broad-area announcements into DOE to fund GTL1, allowing competition among the national laboratories, universities, and private industries. A new FFRDC will not be necessary for this facility.

For the Rare-Isotope Accelerator, R&D is under way, and a request for proposals will be issued in December. A new FFRDC is being created for this facility.

The ILC is not listed here because it was not known whether the architecture would be warm or cold. Now, a cold linac has been selected. CERN is pushing the Compact Linear Collider (CLIC), forcing the United States to compete for this machine. An international forum is needed to discuss such international needs. Unfortunately, the wheel keeps getting reinvented.

The Secretary has been very concerned with the need for education in science. Postdoctoral programs will be continued. Science dropped the ball in middle school, as shown by test scores. The Department of Education is doing its part, and DOE is using its available resources as best it can.

Williams asked whether, under this new method, this research would be competed out to the private sector. Orbach replied, yes.

El-Sayed pointed out that other countries are moving faster in science and engineering education. More publications are originating in foreign countries. More foreign students are returning home after completing their education in the United States. Orbach responded that China is, indeed, meeting our offers to students. That is why the United States needs the facilities. Those facilities keep the United States in front. DOE's science leadership will be decisive. The Earth Simulator woke up the U.S. computing community. The United States can be responsive, but it is going to be competitively tough. Education is our Achilles heel. DOE is trying to deal with it, but needs help.

Stupp noted that Dehmer had said that more coordination between universities and the national laboratories is needed and asked what the intent is in that regard. Dehmer answered that the desire is to make the national laboratories a greater part of the future of U.S. science and to make facilities available to more users from the university communities. Orbach added that the universities are where education advance takes place. DOE wants the national laboratories to support that advance through faculty

sabbaticals and other components of an educational component of the budget. The NSF budget for this is $700 million; DOE's is less than $7 million.

Greene asked if it were hard to get an overview of the health of science in the United States and asked how the increase at DOE balances with the decrease at NSF. Orbach replied that Looney will talk to that point in his presentation later in the meeting. It is not only NSF but also the National Institute of Standards and Technology (NIST) and other agencies. The EU is thinking of a single agency for funding science. That has some real dangers associated with it. The diversity of funding in the United States has strengths; but the health of the whole complex requires all agencies to be adequately funded.

Gates asked how science is becoming globalized. Orbach responded that the United States no longer has a corner on the market for science education. Science leadership translates rapidly into economic consequences. China has a space program and will use it for space exploration. Taiwan's investment in nanotechnology is very significant. The United States' nanocenters are picking up on unique opportunities, and other countries will do that also in the future.

Stupp asked how an intervention could be made at the federal level to have a dialogue on outsourcing. Orbach noted that it is a competitive world. The United States has done pretty well. We have a responsibility as a society to compete. The United States can be the very best in facilities. The Chinese, Japanese, and EU have said they cannot plan facilities as we have in the 20-year facilities outlook. They need committee decisions. SC took Committee advice and acted on it. Cross-field committees often fall apart because of argumentation among the committee members from disparate fields. The United States is the only country to have accomplished this.

A break was declared at 10:46 a.m. The committee was called back into session at 11:10 a.m. Hemminger asked **Walter Stevens** to provide an update on the plans for a second COV for the Chemical Sciences, Geosciences, and Biosciences Division.

That visit is scheduled for April 6-8, 2005, and is to be chaired by Gordon Brown of Stanford University. On an organization chart, Stevens pointed out the new members of the division and the new sections of the division that were not reviewed in the prior COV.

The charge to the Committee was to (1) assess the efficiency and quality of the processes used to solicit, review, recommend, and document proposal actions and to monitor active projects and programs for both the DOE laboratory projects and the university projects and (2) comment on how the award process has affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements within the boundaries defined by DOE missions and available funding. A new portion of the COV is to provide input for the OMB evaluation of BES progress toward the long-term goals specified in the OMB Program Assessment Rating Tool (PART). Each of the nine components (or subcomponents, if appropriate) of the Chemical Sciences, Geosciences, and Biosciences Division were to be evaluated against each of the four PART long-term goals.

The PART states that, by 2015, BES is to demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials, and more (particularly at the nanoscale) for energy-related applications.

It is also to demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy-transfer processes.

It is also to develop new concepts and improve existing methods for solar energy conversion and other major energy-research needs.

It is also to demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

For each of these goals, the COV will be asked to note how each of the components of the division contributed to the achievement of these goals. The Division's performance in striving toward each of these goals is to be characterized as excellent, minimally effective, or insufficient.

"Success" is attained when BES-supported research leads to important discoveries that impact the course of others' research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries. "Minimally Effective" is defined as being when BES-supported research leads to a steady stream of outputs of good quality. Expert review (this COV) every three years will rate the progress of the Division toward its goals using these definitions.

The COV was divided into six subpanels. The first will review Atomic, Molecular, and Optical Science and Chemical Physics. The second will review Photochemistry and Radiation Research. The third will review Catalysis and Chemical Transformation. The fourth will review Chemical Energy and Chemical Engineering, Separations and Analyses, and Heavy Element Chemistry. The fifth will review Energy Biosciences. And the sixth will review Geosciences.

A balance will be struck in the membership of each subpanel between universities and national laboratories and between funded and nonfunded researchers. Greater credibility should result from the inclusion of nonfunded principal investigators. Each subpanel was assigned a chair, and invitations were issued partly based on the chairs' suggestions.

The visit will cover 2.5 days. The first day will be taken up with a division overview, first-read subpanels, a COV executive session, a COV/BES management meeting, and a dinner. The second day will be taken up with second-read subpanels (the panels will be mixed up, but the chairs will remain the same), a COV/BES management meeting, a first/second read merge, and a working dinner. The third day will be taken up with a COV executive session, the drafting of a final report, and a closeout session with BES management. More time may be needed for discussions with senior management. The staff is looking at what material should be supplied to the COV members. The panel needs to delineate recommendations and findings so they can be responded to.

Bucksbaum inquired whether the OMB is interested in the entire report or just the report card. Stevens replied that the whole report will go to them. Bucksbaum asked if someone from OMB will be in attendance during the visit. Stevens responded that that has not been done in the past. Hemminger observed that it is a BESAC report; there should not be an OMB representative.

Gates asked what the executive presentations would include. Stevens responded that they would cover what has been planned, what has been accomplished, and what would make a strong portfolio.

A lunch was scheduled for the BESAC members so that they could learn about the new requirements for and on advisory committees and their members. The meeting was adjourned for that lunch at 11:32 a.m. During lunch, the Committee members were

addressed by Gloria Sulton about changes in the relationships between advisory-committee members and the federal government.

Monday, December 6, Afternoon Session

The meeting was called back into session at 1:35 p.m. Hemminger rearranged the agenda and introduced **Patrick Looney**, OSTP, to talk about "how the government works." (Who OSTP is, the strategic context for R&D programs, macroeconomics of the budget, administration priorities, and some current activities.)

The OSTP mission is to advise the President [and by implication, the rest of the Executive Office of the President (EOP)] and to lead an interagency effort to develop broad S&T policies and budgets. It has two advisory committees of its own: the President's Council of Advisors on Science and Technology (PCAST) and the President's Information Technology Advisory Committee (PITAC). They produce high-level-input reports. OSTP also chairs an Intergovernmental Policy Council, the National Science and Technology Council (NSTC), which allows agencies to come together to discuss broad S&T issues.

Society makes demands on the scientific disciplines to support defense, energy, economic security, health, the environment, food and water, and discovery. Science offers a variety of opportunities. The balance between these demands and the opportunities leads to a budget document.

At the highest levels, the questions that come up are:

- How does the science benefit society (which is centered around jobs, economy, defense, etc.)?
- How does this alleviate/placate constituent concerns (which are aimed at Congress)?
- How has the program been managing and performing (which has a large agenda in this administration)?
- What have we gotten for our investment to date?

At every level, people have different questions and interpretations.

The FY05 proposed budget for the entire federal government amounts to $2.4 trillion. Mandatory spending accounts for two-thirds of the budget and includes Medicare, Medicaid, other mandatory programs, Social Security, and interest payments. About half of the rest of the budget goes to defense. As a result, the United States Government can be looked upon as an insurance company that has an army.

Historically, R&D spending tracks the full budget, and most R&D expenditures are driven by defense R&D. R&D as a share of discretionary spending has been approximately constant for the past 30 years. The budget is currently in a deficit situation, producing serious budget constraints, and there is great uncertainty looking forward. There will be significant pressure on the discretionary budget. R&D will capture 11% to 14% of the discretionary budget annually (up, down, or flat). Appropriate emphasis on science for the public good will continue and probably grow. The large-scale mix of investments will change in response to societal issues and concerns. (In the 1960s it was space, in the 1970s it was energy, in the 1980s it was defense, in the 1990s it was health, and in the 2000s it is homeland security. In the future, it might be energy again.)

The budget will emphasize R&D investments that lead to innovation, job creation, and economic strength. It will also emphasize performance and management of R&D programs. There is already a greater emphasis by the Administration and Congress on understanding what we are getting for our investment and on maximizing return on the large existing investment base. The question is being asked, "How are things managed?"

There is a bewildering array of new facilities being recommended, more than can be funded under the most optimistic budget scenarios (by a factor of 2 to 4). In addition, there is a chronic tension among new and existing facilities. Sustainability of the research programs will force a debate on the future of facilities and the laboratories that house them. There is a need to find graceful end-of-life pathways for aging facilities. In a tight budget era, only the most deserving facilities will be fundable. Reviewers will look at scientific impact (breadth and depth) and the nature of discovery. A national imperative will be the driver, not regional needs or stewardship.

The presidential priorities in this administration are

- Winning the war on terrorism,
- Securing the homeland,
- Strengthening the economy,
- Developing a national energy strategy, and
- Improving government, as stated in the President's Management Agenda and its R&D Investment Criteria and PART Analysis,

although these categories do not capture everything.

Of the five major priorities in FY05 R&D, many align with the administration's priorities:

- R&D for homeland and national security
- Networking and Information Technology R&D (NITRD; which includes scientific computing)
- Nanotechnology
- Molecular-level understanding of life processes
- Environment and energy (including climate change, environmental observations, and hydrogen R&D)

The FY06 R&D priorities add a new one in the number four position: priorities for the physical sciences. Priority will be given to research that aims to close significant gaps in the fundamental *physical understanding* of phenomena (not new technologies) and promises significant new technologies with broad societal impact: superconductors, molecular electronics, quantum condensates, spintronics, etc. Priority will also be given to those instrument- or facility-related investments with the greatest promise for the broadest scientific impact. Of particular interest are investments leading to the development of next-generation light sources in a coordinated fashion. In the physical sciences, priority will be given to those projects and programs that are demonstrably well coordinated with related programs in other agencies or other countries, as described in the interagency working group report, *A 21st Century Frontier for Discovery: The Physics of the Universe*.

Today, the frontiers of the large and the small remain unconquered. But they have receded so far from the world of human action that the details of their phenomena are no longer very relevant to practical affairs. Society will continue to support exploration of

the traditional fields of the large and the small, but will do so with increasing insistence on careful planning, management, and sharing of costs.

The physical sciences lacked a vision for discovery until the report *Quarks to the Cosmos* was issued. There, a compelling case for science was articulated in the form of questions. The stated case was agency- and program-independent, with NASA, NSF, and DOE all having a role. This report provides an intellectual framework for R&D in the physical sciences:

- What is the dark matter?
- What is dark energy?
- How did the universe begin?
- Did Einstein have the last word on gravity?
- Etc.

Looney used an organization chart to show the many committees that exist under the NSTC. In response to the *Quarks to the Cosmos* report, an interagency working group (IWG) was formed, with NASA, NSF, and DOE making up the membership. That group analyzed the different scientific problems identified in *Quarks to the Cosmos* and identified the scientific approaches that could be taken to arrive at answers to those problems. The scientific approaches were grouped by stage of maturity, ranging from "ready for immediate investment" to "things we need more information about." The items ready for immediate investment are priorities in the FY06 budget.

The NSTC also has an IWG looking at materials characterization facilities. That group issued a report in 2002 that noted that the United States is source poor, the SNS is the only new neutron source on the horizon, there is a need to maximize existing facilities, and instrument development is needed for the SNS.

Isaacs commented that it looks like OSTP is in charge of DOE facilities. Looney replied that OSTP is just the chair of the IWG. DOE and other agencies are the owners of the facilities. Isaacs noted that any facility or society needs a vision and government needs metrics for judging results. Society is impatient for results. The government seems to have some role in shortening the timescale for results. Looney said that OSTP is not interested in the time scale or the instruments needed to get the results. One cannot guarantee results, but one can discuss how to go there.

Plummer asked what he had meant by a lack of vision for discovery. Looney took as an example an investment in deep-space telescopy and asked how it is related to particle physics. No single picture is available to show how the two fit together.

Isaacs observed that industry has pulled back from funding research and asked if that was the view of OSTP and, if so, what has to be done to compensate for it. Looney answered that OSTP does recognize such a pullback. It is not sure what has to be done nationally but knows that it will involve the national laboratories (e.g., centers of excellence). Gates asked if there is debate about the issue. Looney responded affirmatively.

Berrah asked who would address the questions about materials characterization listed in the last viewgraph. Looney said that an IWG subcommittee is to look at those questions. Some of the answers lie in BESAC and other reports but need to be pulled together to fill in the gaps.

Kohn asked him about the U.S. position on the scientific aspects of global warming. (Global warming is too economically burdensome and scientifically unproved.) Looney

responded that the Administration has since accepted the National Academy report results. Kohn noted that the UK Prime Minister has accepted the reality of global warming and its eventual consequences and that it is the number one priority of the Group of Eight. Moreover, Russia has signed the Kyoto Protocol. He asked what OSTP is doing about the science. Looney replied that Earth observation is a high priority. There is a belief that a heavy investment must be made in technologies that do not emit radiatively active gases. It is incorrect to believe that the United States does not ascribe to the Kyoto Protocol in any way.

Hemminger introduced **Michael Lubell** to "tell us the future." Lubell said that he did not know what the future will hold but would reflect on a few issues.

Based on exit polls, the five hot issues in the recent election were terrorism, the Iraq war, the economy and jobs, health care, and moral values. A postelection issue poll indicated that people voted on the basis of national security, domestic issues, and moral values (25%).

Similar polls indicate that scientists are seen as elitist, arrogant, liberal, Democrat, and out of touch with middle America. Science is considered by many as an enemy of the Bush administration (in terms of the Kyoto Protocol, ABM Treaty, stem-cell research, evolution vs. creationism, the Union of Concerned Scientists' reports, and the fact that scientists stand for change). Half of the U.S. population does not believe in evolution. These views have put the scientific community at odds with the White House; this does not bode well for science or the country.

Science needs to build bridges to the public. More than 85% of people polled believe that science is beneficial, but only 20% of the people polled named jobs and the economy as a principal benefit. Fewer than 10% could name any place where research is performed. Science also needs to build bridges to the White House to repair the damage by speaking the language, engaging industrial allies (they are interested in the fruits of basic and applied research and in the workforce), and encouraging conservative scientists to speak out.

The country faces a series of budgetary challenges. It has a structural deficit, a historic current accounts deficit (the Social Security surplus is going to vanish), foreign ownership of federal debt (92% during the past 4 years), a sinking dollar and rising interest rates, entitlement pressures for Social Security and Medicare (two-thirds of the budget), tax cuts, the Iraq war, and homeland-security costs. These issues will continue to get a lot of budgetary attention. The on-budget (without Social Security) deficit will be exceedingly large for the foreseeable future.

The timeline for the FY07 Budget is

- Spring 2005: OMB guidance to agencies
- Summer 2005: Agency planning
- September 2005: Agency requests submitted to OMB
- Thanksgiving 2005: OMB "passbacks" sent to agencies
- January 2006: Presidential Request finalized
- Feb. 6, 2006: Presidential Budget submitted to Congress
- April 15, 2006: Budget resolution is supposed to be passed by Congress
- Spring and Summer 2006: 13 appropriations bills passed by House
- Spring and Summer 2006: 13 appropriations bills passed by Senate
- Summer 2006: 13 appropriations bills conferenced

- Sept. 30, 2006: 13 appropriations bills passed and signed into law (or a continuing resolution signed)
- Oct. 1, 2006: Start of FY 2007

For the future, the only significant growth that is predicted is for the Department of Homeland Security and in the NASA budget to fund the Moon-Mars mission. The inside story of the FY05 budget is that it was passed in 5 hours, with no one reading it. The DOE champions were Hobson, Visclosky, Biggert, Domenici, Reid, Alexander, and Bingaman; the scientific community needs to say thank you to these people. The NSF was caught in a squeeze between veterans (who were potentially underfunded) and Moon-Mars (Tom Delay pressed for more money for NASA; the Moon-Mars mission was added and came out of NSF funding). These are the evils (for NSF) and benefits (for DOE/BES) of an omnibus bill.

A few percentage points of decrease is bad because, to stay the same, one has to have a 2 to 5% increase to meet inflationary costs. A 2% decrease is a 6% decrease in level of effort. Nondefense R&D in the federal budget has stayed about the same for many years now.

The key messages that the scientific community should put forward should be about economic growth and jobs, global competitiveness, national security, health care, and a high-tech workforce. In the early 1970s, when the dollar slipped, there was no single currency that was seen as stable and safe; there is now: the euro. The future should be benchmarked in terms of patents, high-tech-industry output, R&D spending, publications, and student enrollments. These are indicators of where we as a nation stand.

In terms of U.S. patent applications, the United States is still leading the "old" economies by a small margin, but the emerging economies are increasing rapidly. Sometime in the future, the emerging economies will overcome everyone else. Those countries have a huge population and are becoming more educated. Much the same can be said about the high-tech-industry gross output of China; and the R&D spending in emerging economies is experiencing much greater growth than that in the United States. Attention should be paid to R&D as a segment of our spending to produce gross domestic product (GDP). The ratio of federal physical science research funding to GDP has decreased by 50% since 1970. The industrial sector has gotten out of the R&D business, and government needs to step in to maintain the nation's ability to compete.

In terms of papers submitted to *The Physical Review*, submissions from Western Europe and from the rest of the world have grown significantly since 1983; submissions from the United States have remained flat.

In terms of education, the number of U.S. graduate students in engineering, physical sciences, mathematics, and computer sciences in U.S. institutions of higher learning has decreased from about 75,000 to about 65,000 between 1995 and 2001. The number of such graduate students from foreign countries has increased from about 50,000 to about 80,000 during the same period. Burton Richter has said that happy faculty members make happy students; and indeed, the number of bachelor degrees in the physical sciences, mathematics, and engineering tracks closely the number of dollars expended for nonbiomedical federal R&D.

The scientific community must engage the public; everyone in science and technology has to talk to the public. Getting political is very important and is a lifelong battle. Creationists have the same interests in technology, science, and health care as

everybody else. And it must use the power of its numbers; the scientific community is very large.

Gates noted that Lubell had said that industry had stepped back from research and that government needs to step up its research and asked how one makes that connection. Lubell replied that government agencies are being prodded by investment bankers and others. The Cato Institute said that, if the United States does not do it, others will, and then the United States will not need to. The National Association of Manufacturers is heavily involved and will make a good case for government funding of R&D.

McCurdy noted that a case has not been made as it was in the 1950s and 1960s. Lubell responded that the country has become socially more conservative. Those swinging to conservatism should be addressed by us. McCurdy went on to observe that globalization means that an invention here is exploited outside the United States. Ascendancy in invention is not associated with economic growth and health in the United States. Lubell commented that Norman Augustine would say that the first round of exploitation will be domestic. As the technology matures, it will move offshore. Development as a discovery/invention matures goes where labor costs are low and market growth is high. One can only capture market share at the leading edge. McCurdy pointed out that regulatory barriers (e.g., in pharmaceuticals) argue against that pattern of economic exploitation.

Berrah asked if members of the scientific community should wait for a good time to contact congressman. She noted that Europe is very active in areas that the United States is not and asked if his office planning anything to publicize physics. Lubell replied that the American Physical Society has its membership send Congressmen letters year-round, and last year it got 55 congressmen to sign a letter supporting DOE and BES. He suggested sending a letter to the editor praising Congressmen who have supported science. There is also the problem of political payback to deal with.

El-Sayed asked how to get more young people to go into science. Lubell said that he did not have the answer to that. Students follow their teachers. The lowest quartile of college graduates go into teaching and are paid poorly. Parents have also become less involved in their children's education.

Stupp stated that scientific literacy is very low and that that affects our nation's effectiveness. Lubell agreed that there should be a minimum expectation of people's appreciation of science.

A break was declared at 3:17 p.m. The Committee was called back into session at 3:43 p.m, and **Patricia Dehmer** was asked to present an update on the BES Solar Energy Workshop (which will not be a BESAC workshop). She reiterated that it is appropriate to thank the chairs of the appropriations committees. The budgeting challenges are great, but BES needs to do planning for the future. The next follow-on to the Energy Security Workshop will be a workshop on solar energy.

Future world energy needs and solar-energy potentials were discussed at the DOE 2004 Nano-Summit, where Rick Smalley issued his terawatt challenge: nonfossil-fuel-based generation will have to increase from 0.5% of world energy generation in 2003 to about 50% of the generation in 2050. At that same meeting, Nate Lewis review the potentials of renewable energy sources and pointed out that solar energy has the potential of producing 120,000 TW but can only practically produce 600 TW.

Now, a Workshop on Basic Research Needs for Effective Solar Energy Utilization

needs to be held to identify basic research needs and opportunities in solar-electric, fuels, solar-thermal, and related areas, with a focus on new, emerging, and scientifically challenging areas that have the potential to have significant impact in science and technology. It will look at processes to overcome short-term showstoppers and long-term grand challenges for the effective use of solar energy. Lewis has agreed to chair the workshop with George Crabtree as the co-chair.

The workshop will have breakout panels and subpanels on solar electric, solar fuels, and cross-cutting issues. It is scheduled for April 18-20, 2005, at the Bethesda North Marriott Hotel and Conference Center. On April 21, a report will be written by a core group. A plenary session will include overview presentations by representatives from DOE technology programs, leading industries, and academic institutions. Breakout-panel discussions will be grouped by subpanel topics. Each subpanel will have about 12 members, consisting of leading experts from the United States and foreign countries. Two observers from each DOE laboratory will also be invited to attend the workshop. BES will provide financial and administrative support to the workshop.

Planning has been coordinated with the DOE–EERE Solar Technology Program. EERE staff will provide to panelists pre-workshop briefings on critical solar-electric and solar-thermal research needs.

Prior to the workshop, a document will be prepared summarizing the current developments in each breakout session. It will serve as the factual part of the final workshop report, and it will also be used to educate participants prior to the workshop. During the workshop, each panel is expected to generate three to ten high-priority research topics describing key research objectives that would enable revolutionary progress in the field. The workshop report is expected to be published by August 2005. The workshop output will be used by BES for use in laying the foundations for new directions and funding support for research on the use of solar energy.

The timeline for organizing the workshop is

- Announce Solar Workshop at BESAC 08/04
- Issue charge and confirm chair/co-chair invitation 09/04
- Draft workshop outline and confirmed logistics 10/04
- Confirm breakout panel chairs 11/04
- Confirm subpanel chairs and issue panelist invitations 12/04
- Conduct DOE-EERE preworkshop briefings 01/05
- Finalize factual document 02/05
- Issue final agenda and invitation letters 03/05
- Conduct workshop 04/05
- Prepare workshop report 05-06/05
- Finalize draft workshop report 07/05
- Submit workshop report to BES 08/04
- Disseminate report and start community outreach 09/04

All BESAC members are invited to participate in the workshop and will receive a formal invitation.

Kohn noted that, in the near term, solar energy can have a big impact on the off-grid population with little capital investment. It would be good to have someone talk about the economic aspects of solar energy in the near and long terms. The leader in solar energy research is Japan, where subsidies are provided until economies of scale kick in. The

workshop should include a review of research in Japan. Dehmer said that the organizers of the Hydrogen-Economy Workshop plan to do that and that this is going to be a big workshop. Stevens commented that the workshop would survey all the technologies applicable to solar-energy production.

Hemminger asked **Patricia Dehmer** to initiate a discussion on BES grand challenges. Dehmer gave examples of discovery-class science in BES:

- Can we understand, model, and predict the fundamental phases of matter (including liquid crystals, plasmas, condensates, superfluids, etc.)?
- What is beyond the "standard model"?
- What is the nature of the chemical bond?
- How do e-atomic molecules, cells, and organisms naturally communicate?
- Are there undiscovered organizing principles at the nanoscopic and mesoscopic scales?
- To what extent are reductionist approaches to phenomena limited?
- What are the molecular origins of the evolution of life?

Bucksbaum noted that these grand challenges need to be integrated with the needs of society. An organization like BES with its large and small laboratories and programs needs to be brought to bear on the needs of society. BES can really help with discerning the costs and benefits. Dehmer replied that BES is a strong research organization with strong ties with society. Its workshops are highly focused on the needs of society. As a result, it has a problem getting the community to move outside the box they are trapped in. These talks should be bound together to produce a broader perspective. Bucksbaum continued that far-out things should be thought about. Encouragement is also needed to bring different expertises together to see their commonalities and to address problems in a unified manner.

Kohn commented that a meeting in France a couple of years ago addressed chemical bonding and polarization of hydrogen bonding. That phenomenon has tremendous potential for further development. El-Sayed pointed out that weak interactions need to be understood, not just strongly polarized bonds. Stupp pointed out that an immature area is the physics of supermolecular chemistry. It governs biological processes and represents a gap. It is difficult to grab ahold of. Computational simulations can help. This problem brings together many fields. Morse stated that many scientists are working on such problems that are poorly understood but very efficient and, therefore, important.

Williams put forward the questions, "What is a photon? How do they react with matter and other photons?" He pointed out that new experimental and theoretical tools (e.g., slowing light down to study this question) are available and that those questions represent a new and fertile field.

Gates stated that everyone can learn from nature down to the molecular level.

Hemminger asserted that the comment on the reductionist approach seems heretical. Morse offered that it could have come from the Office of Faith-Based Initiatives. Systems biology is focusing on exactly that area, and it will resonate with current funding areas at NSF and the National Institutes of Health (NIH) as well as with engineering.

Kohn said that "reductionist approaches" brought to mind emergent and collective properties and asked if they were the same. Dehmer replied, no.

Plummer noted that a number had used a term twice that half the population does not believe in. Greene explained that what a chemist calls phase transition is not what a

physicist would call phase transition. Scientists should learn how to communicate better between chemists and physicists. They can learn a lot from each other. Williams pointed out that the generalization of architecture means building large computer systems. These architects can contribute a lot to each other and to those who study biological systems. However, it takes years of exposure to get to the point where meaningful communications can take place.

El-Sayed suggested that the interphase at the molecular and atomic level might be a fruitful area of inquiry.

McCurdy stated that reductionism can mean different things to different scientists and to classical philosophers. There is something "not sharp" about that bulleted item.

Hemminger asked for public comment. Helen Farrell suggested that it may not be appropriate for people at national laboratories to thank the congressional committee chairs. Dehmer concurred. There being no other public comment, Hemminger adjourned the meeting for the day at 4:31 p.m.

Tuesday, December 7

Chairman Hemminger called the meeting to order at 8:33 a.m. He asked the Subcommittee on Theory and Computation to present its draft final report. **William McCurdy** led off the presentation.

The Subcommittee received the charge to identify current and emerging challenges and opportunities for theoretical research within the scientific mission of BES, paying particular attention to how computing will be employed to enable that research. A primary purpose of the Subcommittee is to identify those investments that are necessary to ensure that theoretical research will have maximum impact in the areas of importance to BES.

The first meeting of the Subcommittee was held on February 22, 2004, prior to the February meeting of BESAC. On April 17-18, the Subcommittee met in Chicago to take testimony and to discuss preliminary ideas and findings, following the process of an National Research Council committee. From this meeting, the Subcommittee got an idea of what the principal directions should be and developed an outline. A website was established for written testimony in March. On June 4, a letter report of the Subcommittee was delivered to John Hemminger and Pat Dehmer for discussion at the August meeting of BESAC. On July 30, the first draft "extended outline" was delivered to the entire Subcommittee. On August 5-6, BESAC discussed the preliminary report. On October 9, the Subcommittee met in Denver to discuss its findings and recommendations. In October and November, it assembled, edited, and circulated drafts. On December 6-7, it presented the proposed final draft to BESAC. In January 2005, the final bound report will be delivered to SC and to BES.

The Subcommittee members were listed, and an outline of the report was presented:

- A confluence of scientific opportunities: Why invest now in theory and computation (T&C) in the basic energy sciences?
- The unity of T&C in the basic energy sciences
- BES community input and assessment
- Emerging themes in BES: Complexity and control

- Connecting theory with experiment in BES: Accelerating discoveries and furthering understanding
- The resources essential for success in the BES theory enterprise
- Findings and recommendations

The early parts of this outline address the basic syllogism of why now is the time to invest in T&C and they underscore that T&C are not separate activities. The remainder of the outline lists nine opportunities offered by T&C.

Four developments have happened that amplify the capability of theory to influence the advance of science:

- Striking recent scientific successes of theory and modeling;
- The appearance of specific new scientific frontiers, such as nanoscience and biomimetics;
- The construction of new experimental facilities and the development of new small-scale experimental capabilities; and
- The massive jump in computational power, including the promise of new leadership-scale computational facilities.

McCurdy turned the floor over to **Kate Kirby**.

The unanimous view of the Subcommittee was that theory and computation should be considered one and the same. Often, there is no clear distinction between conceptual theory and the formulation of mathematical models. Theory enterprise is heterogeneous, with regard to group size, the required computational resources, and whether the research is a single-PI or multiple-PI effort. BES needs to support the complete spectrum of T&C.

The report goes on to consider growing a balanced program. This is an important concern of the Subcommittee as well as of the community. There has been a growth in the BES facilities budget, but *no* such growth in the BES core research programs. The Subcommittee is concerned that new investments in BES T&C be balanced between the core program and facilities.

The research in BES is extremely diverse, which is a tremendous strength. However, that diversity makes it difficult to organize the subject matter. The Subcommittee identified two overarching themes characterizing the science: complexity (several electrons, atoms, etc.) and control (variables that can be tweaked). The ultimate goal is to control complex systems.

The opportunities and challenges in complex systems include nanoscience (e.g., extremely small medical technologies that have captured the imagination); correlated electrons in solids (which are important for magnetic applications); electronically excited states (which play key roles in photosynthesis and other systems); and defects in solids (that greatly affect material properties and need to be understood in terms of their microstructural defect states).

The opportunities and challenges in quantum control include the control of energy, matter, and information at the quantum level (e.g., ultracold degenerate gases); ultrafast physics and chemistry (where quantum control is exercised through custom-selected radiation, such as by fourth-generation light sources at ever-shorter light pulses); and magnetic spin systems and single-electron devices (e.g., molecular-electronic junctions, which hold promise for the miniaturization of electronic devices).

The opportunities and challenges in the control of complex systems include biomimetic materials and energy processes (which offers the efficient conversion of light

energy, promises new sources of energy supply, and overlaps with nanotechnology) and the control of chemical transformations (which covers all chemical reactions, including catalytic processes).

Taylor commented that modeling seems to be downplayed here and asked if it had taken on a new meaning. Kirby replied that the Subcommittee had considered modeling part of computation and theory; it was not trying to ignore the topic. McCurdy added that the Subcommittee could not agree what "modeling" means and whether it is different from simulation. So it referred to T&C and avoided the distinction.

El-Sayed said that the illustrations point to the importance of nanostructure. Bucksbaum commented that the beautiful pictures could have been more informative. They are more important than the text because one looks at them first. They need scale bars and other aids to explicate their meaning.

Gates offered that there are opportunities to introduce more concreteness into the report. Suggestions on how theory and computing have advanced science and how they can do so in the future could be added.

Isaacs said that the report needs to show how computing has solved problems and why it is needed for future advances. McCurdy stated that the Subcommittee understands that simply greater computing resources are not the answer to some forefront research areas where fundamental theoretical concepts must first be formulated. The need for resources is divided: some research projects need theoretical advances and others need greater calculational power.

Kohn observed that the advisory committee of the ALS has recommended more theoretical support for the users. An important thing happening is the movement to very small size scales. Traditionally, the term "excited states" has meant stationary excited states. But it is now moving into another meaning: a rapidly developing condition of the system. One has to better understand the time factor of the system. One of the bedrocks of chemistry is the Born-Oppenheimer Approximation, which loses its applicability under time-evolving conditions. One must have enormous computing power to deal with it. The time-dependent density functional theory (DFT) looks like it may become very important. It can lead to a great simplification of understanding the movement of massive numbers of particles. Nuclear physicists have been looking at the dynamics of large nuclei in a time-dependent regime. This effort has not been very fruitful. The best they have done (Hartree-Fock) is not very good.

Bruce Harmon continued the presentation. One concern of the Subcommittee was the balance between tabletop science and large facilities. The two methods complement and guide each other.

The Subcommittee also wants to stress the connection of the theory program with the science at existing BES facilities. Huge amounts of data are being produced, and help is needed in interpreting those data. A stronger coupling of T&C with experiments is needed at BES facilities. The new major experimental facilities need theoretical support and guidance in order to ask the right questions and to understand the answers. These new facilities include the five nanoscience facilities, the SNS, and the LCLS. The availability of theoretical advice would go a long way to ensure the success of those facilities.

The resources essential for success in the BES T&C enterprise are (1) the spectrum of computational resources, (2) new styles of support (scientific codes as shared instruments), and (3) human resources (training future generations).

The spectrum of computational resources needed constitutes the "Branscomb pyramid," which includes leadership computers (maybe just one), (several) national supercomputers, (many) university computer clusters, and (ubiquitous) personal computers and workstations. A lot of work is needed at the cluster level to make the problems understandable so they can be addressed by larger machines. Many problems exist that could be effectively addressed by leadership-class computing.

To achieve the ultimate goal of predicting system properties and behavior, robust algorithms and software are needed, particularly at the leadership-class level. These algorithms and software, in turn, need theory to be based on.

Large-scale facilities have large user communities. Large computer facilities need a large community to produce the requisite algorithms and then share them. A lot of these algorithms are now coming from Europe. The most important impact here is human resources. Students and postdoctoral fellows are the lifeblood of BES. U.S. facilities need to attract and support bright young people, who are mostly found in university single-PI groups.

Berrah said that this task is a big challenge, and the Subcommittee is to be congratulated. The human resources are very important. Physics and chemistry departments do not encourage theorists. That culture needs to be changed. She asked if the Subcommittee believes that theorists need to be present at the big facilities to establish a connection between theory and experiment. Harmon responded that there has been a huge growth of theorists in industry in magnetism and biology. The Subcommittee did not have enough information to state whether in-house theory groups would be needed or not. It is not clear when and where interpretation will be needed and how it would be supplied.

Bucksbaum pointed out that the report has no finding about there being an inadequate number or supply of theorists. He asked if this was not the case and what the Subcommittee thought about this situation. McCurdy replied that the findings were voted on early in the process. The report needs to discuss the issue referred to. There is not enough theory being done.

Long asked if the Subcommittee saw a difference between the coupling of theory and experiment at the nanoscience centers and at other facilities. Cummings noted that the nanoscience centers are still a work in progress. The goal is to have theorists onsite to provide support to experimentalists and to other theorists.

Long asked whether anything was discussed about partnerships between universities and national laboratories. Harmon replied, yes, the topic was discussed quite a bit.

Flynn pointed out that an enormous advantage of large computing facilities is that one does not need to go there to use them. He said that he would like to see the report emphasize this advantage and the need to optimize the remote access to those facilities.

Isaacs noted that it is a big deal to develop community code; it is a massive effort. BES can support such an effort, and others cannot. Such development can also be done over a network. Hammond agreed, pointing out that (1) there are such networks and (2) that concept could be expanded to develop robust code.

Kohn considered the question of whether there should be theorists on the premises or

not. In the fifties and sixties (of the past century) at the high point of the Bell Labs culture, that organization had world-class theorists onsite. There was an understanding that these theorists were available for discussion and consultation but were also expected to do "their own thing" at the same time. The balance between those two activities was not quantitatively determined. There was effective intercommunication.

Berrah stated that the report needs to emphasize the need for a balanced distribution of theorists across the research landscape.

Stevens noted that the idea of software development has been difficult to get continued funding for. There are several paradigms: development of software for in-house use (but, generally, that software is not maintained well); a commercial enterprise; and a self-assembly in the public domain of a network of open-architecture codes. BES needs to think seriously about how to develop such software.

McCurdy resumed leadership of the discussion. In the draft report, the findings and recommendations are presented in coupled sets.

The essential finding is that regarding T&C in BES. During the past decade, the facilities budget has grown strongly but has been associated with essentially no increase in support for T&C. The core programs have effectively decreased, and theory and computation have decreased along with them. Consequently, opportunities have been missed, including some at the facilities themselves. This trend has also disadvantaged many innovative individual experimental efforts in universities and the laboratories with which those theory efforts have been coupled. The Subcommittee recommends an initiative to increase the BES efforts in T&C. This assertion is elaborated on by the rest of the findings and recommendations.

The Subcommittee found that new opportunities for T&C have been created by a recent confluence of striking scientific successes and the appearance of specific new scientific frontiers. It has identified nine areas of opportunity, spanning the range of the BES portfolio:

- Nanoscience
- Correlated electrons in solids
- Electronically excited states
- Defects in solids
- Control of energy, matter, and information at the quantum level
- Ultrafast physics and chemistry
- Magnetic spin systems and single-electron devices
- Biomimetic materials and energy processes
- Control of chemical transformations

This list is not exhaustive. The Subcommittee can make a compelling argument at least in these topics for a major effort in theory. It recommends (1) that, in all of these areas of opportunity, progress would be greatly accelerated by advances in fundamental theory to develop new paradigms to solve those problems and (2) that BES should invest in such research. In many of these areas, new, fundamental, conceptual theory is essential to progress. The ultra-intense X-ray sources will make no progress without theory. The Subcommittee also recommends that, because a number of these areas are poised to exploit high-end computation (especially nanoscience, chemical transformations, electronically excited states, defects in solids, and correlated electrons in solids), investments should be made to ensure the expansion of such computationally intensive

research. Computation in these areas is essential to establishing and maintaining a leadership role for BES in both theoretical and experimental facets of these disciplines. Computation is essential. Codes are already available in many cases.

The Subcommittee found that science does not know all the equations, nor does it have all the mathematics and physical insights needed. Therefore, all the algorithms needed to solve the research problems in the BES portfolio have not yet been invented. Without new algorithms and concepts, no computer will solve the problems. Many of these problems do not scale. The Subcommittee recommends that conceptual theory not be viewed as a separate enterprise.

The Subcommittee found a recent trend in certain BES programs (for example at the Nanoscale Science Research Centers) to increase the coupling of theoretical and experimental activities. This coupling is both proper and timely. It is wonderful, but, at the existing light and neutron sources, there appears to be little conscious or systematic effort by BES to stimulate and support, with targeted resources, theoretical partnerships with experimental efforts. We believe that this situation puts at risk DOE's ability to extract the maximum scientific benefit from those facilities. At the facilities currently under construction (the Nanoscale Science Research Centers and the Spallation Neutron Source), some efforts have been made to incorporate theory into the planning for the facilities. These efforts are uneven at best and certainly incomplete. The Subcommittee recommends that BES should undertake a major new thrust to significantly augment its theoretical and computational programs coupled to experimental research at its major facilities. When new experimental facilities (e.g., the LCLS) are proposed by BES, the associated theory and computational efforts should be incorporated from the outset. At its existing facilities, BES, with support of user groups, should upgrade the theory and computations associated with experimental programs. BES cannot do it over the heads of the user groups. The solution will be different for each facility. Increased investments in the BES programs are needed to build theory efforts that strongly couple to science at existing facilities. In the Subcommittee's process, the coupling of desktop and large facilities came later.

On computational resources, the Subcommittee found that (1) BES is ready for and requires access to leadership-scale computing to perform calculations that cannot be done elsewhere and (2) a large amount of essential BES computation falls between the leadership scale and the desktop scale. The Subcommittee recommends that BES should become strongly engaged with the DOE Office of Advanced Scientific Computing Research to ensure that large amounts of time on terascale capacity facilities are available to the BES scientific community. Also, BES should consider supporting some of this capacity with local institutional computing, while ensuring that demand at the higher end of computing power is supplied by larger facilities. BES has three times the number of requests that can be accommodated. The capacity capability must be addressed.

For years, NIH has been paying technicians to upgrade, harden, and maintain code and infrastructure. BES should support the development and maintenance of scientific codes in the disciplines in its portfolio, just as it now funds the development of shared beamlines at its experimental facilities, thereby creating new scientific capabilities for the nation. Such investments will also be critical in allowing BES researchers to take full advantage of the capabilities of DOE's leadership-class computing facilities.

These are the findings and recommendations as they now stand.

Hemminger asked the Subcommittee cochairs to elaborate on the discussions that had been held and how they affect the findings and recommendations. McCurdy said that the Subcommittee included two experimentalists to keep it honest. Carl Lineberger said that there was a concern in the experimental community that the report will not say that benchtop and large-scale facilities are both important and must be complementarily supported. There is no recommendation along those lines. A recommendation should be included to the effect that increased support for T&C should enhance T&C connections not only to the large experimental facilities but also to forefront experimental tabletop science directly relevant to DOE.

Plummer said that he believed that this issue is very important. In the end, this report advocates allocating nonfacility money into theory. He did not believe that that case had been made. Some would say let NIH and NSF support the theory. But one cannot advance microscopy without theoretical support at all levels. The tools are available, but the users do not know how to interpret the pictures. The National Nanotechnology Initiative (NNI) will not achieve its goals without theoretical support. McCurdy stated the case more bluntly: If one takes away support for benchtop research, one will not need theorists. Plummer commented that, in nanotechnology, the many scanning-probe techniques are strongly dependent on T&C for the interpretation of the acquired data. McCurdy acknowledged that the Subcommittee had missed that argument, which makes a powerful case for theory in the nanoscience program.

Hemminger said that a compelling case is made in this document. There are things that could be added. But not every application should be listed. The report may be further along than Plummer's comments would imply.

Bucksbaum commented that the report needs a statement that not enough effort and people are devoted to theory in the frontier areas of science. Kirby countered that one does not want to train theorists for whom there are no positions. Bucksbaum continued, this is a finding, not a recommendation. The recommendation would be to increase the resources. McCurdy restated the finding as, there are (1) an insufficient number of theorists and (2) an insufficient amount of effort in theory devoted to the frontier areas of the BES portfolio.

El-Sayed suggested that it might be useful to cite the number of students studying to be theorists and questioned whether students even hear about theory as a career path.

Berrah suggested wording the recommendation as follows: There is a strong need to train and fund theorists at universities and national laboratories to address the scientific areas of the BES portfolio. The Office should seek new initiatives that would provide funding for T&C just as it does for new facilities.

Flynn commented that he had a lot of theorists in his laboratory. They overwhelmingly work on NIH problems. If it is desired to have theorists work on BES problems, resources need to be made available for them. McCurdy agreed and said that he wanted a paragraph about such a need inserted in the report.

Cummings concurred with Flynn, saying that approximately half of his funding comes from NIH. The opportunities for theorists in industry are in pharmaceuticals. Flynn added that there is a commercial aspect to it, also. Where there are commercial spinoffs, there are financial rewards.

Lineberger noted that the section on tabletop science was written rapidly and late in

the process; it should be reflected in the findings. Benchtop experiments are driving innovations, and the coupling of benchtop experiments with theory is crucial. One must continue and accelerate the involvement of theorists in state-of-the-art experiments.

Gates called attention to the fact that not everything is in the report. Maybe one should say that it is not known how to do some of these tasks and that pilot programs should be conducted to see what works.

McCurdy checked to make sure that Lineberger had volunteered to wordsmith the finding and recommendation on benchtop experiments. Hemminger said that that was what he had heard.

Plummer asked why new money could not be earmarked for setting up a code/theory user facility. Dunning responded that some projects have already earmarked such funds. Funding of theory was part of the Environmental and Molecular Sciences Laboratory (a user facility) from the beginning. And when ORNL put in its proposal for the National Leadership Computing Facility, it included the concept of computational end stations to do many of the types of activities that are being referred to here.

Williams noted that students follow the money. Since 1996, he had hired 32 staff members, 31 of whom were from outside the United States. This year, five out of five interviewees were from the United States. The NNI has made this area of science visible and has brought a lot of bright students into it. The NNI made it sexy to go into this area, and he was now seeing the fruits of this effort. If theory is important, one must take a stand for it and also make it obvious that the support is not a flash in the pan but is going to be part of the institution.

Bucksbaum pointed out that theory in BES is not a topic over which to have a turf battle. No matter where the resources come from, the increase in theory will benefit everyone. The training and resources must exist. The question of overemphasizing the national laboratories or underemphasizing the national laboratories is not part of the problem.

Dehmer hypothesized about being asked what could be done with extra funding and having to talk about the most important recommendation in this report: Send more money. This is a trite recommendation. The report must lead off with a more powerful argument. The opening statement about the confluence of opportunities is very powerful. McCurdy responded that that was wise advice.

Hemminger suggested that the Committee's suggestions that are agreed upon be integrated into the report, that a revised version be circulated by e-mail, and that an e-mail vote on accepting the report be asked for. Cummings suggested that the Committee should approve the report with the understanding that suggested modifications will be made. Lineberger suggested that the Committee could require the chair's approval of the final version. Plummer stated that he believed that the committee should read and approve the final version because there will be repercussions on other funding. El-Sayed said that this report is not as bad as the catalysis report; he believed that Hemminger's suggestion was the way to go.

The Committee took a straw vote about how to proceed. By a vote of 12 to 4, the Committee decided to have the draft report modified with comments sent by Committee members to the Subcommittee's cochairs by Friday, December 10, 2004. The revised report will be accepted or not by the chairmen in conference with other, interested members of the Committee.

Johnson asked if nanophotonics was included in the report. McCurdy replied, no. It was missed; a paragraph will be inserted about it.

Hemminger noted that the adopted process should have the report issued by January. Gates asked him to summarize the major suggestions for modifications. Hemminger replied:

1. The leadoff finding and recommendation need to express a compelling need for investment in this area.
2. Justifications are to be inserted for nanophotonics and scanning probes.
3. The illustrations and their captions should have their information content optimized.
4. A finding and a recommendation are to be inserted that (1) acknowledge that innovation at the benchtop level drives innovations at facilities and (2) call for commensurate funding for theory support for benchtop experimentalists.
5. The issue is to be raised about the need for enough theorists and theoretical effort at frontier areas.

Hemminger called for public comment. There being none, he adjourned the meeting at 11:12 a.m.