Minutes for the
Basic Energy Sciences Advisory Committee Meeting
August 5-6, 2004
DoubleTree Hotel and Conference Center, Rockville, Md.

BESAC members present:

- Nora Berrah
- Philip Bucksbaum
- Sue Clarke
- Peter Cummings
- George Flynn (Thursday only)
- Bruce Gates
- John Hemminger, Chairman
- Eric Isaacs
- Anthony Johnson
- Kate Kirby
- Walter Kohn
- Gabrielle Long
- William McCurdy, Jr.
- Martin Moskovits
- Ward Plummer
- John Richards
- Samuel Stupp (Thursday only)
- Stanley Williams

BESAC members absent:

- Mostafa El-Sayed
- Laura Greene
- Daniel Morse
- Richard Smalley
- Kathleen Taylor
- Mary Wirth

Also participating:

- Altaf Carim, Office of Basic Energy Sciences, USDOE
- James Decker, Principal Deputy Director, Office of Science, USDOE
- Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
- Bruce Harmon, Deputy Director, Ames Laboratory
- William Johnston, ESnet Senior Scientist, Lawrence Berkeley National Laboratory
- Dale D. Koelling, Program Manager, Basic Energy Sciences, USDOE
- Frederick M. O'Hara, Jr., BESAC Recording Secretary
- Douglas Ray, Director, Chemical Sciences Division, Pacific Northwest National Laboratory
- Mary-Anne Scott, Office of Advanced Scientific Computing, USDOE
- Rachel Smith, Oak Ridge Institute for Science and Education
- Walter Stevens, Office of Basic Energy Sciences, USDOE
- Karen Talamini, Office of Basic Energy Sciences, USDOE

About 90 others were in attendance in the course of the meeting.

Thursday, August 5, 2004
Morning Session

John Hemminger called the meeting to order at 8:54 a.m. Rachel Smith of the Oak Ridge Institute for Science and Education (ORISE) made safety and convenience announcements. Hemminger asked the committee members to introduce themselves.

Hemminger introduced **Patricia Dehmer** to give an update on the Office of Basic Energy Sciences (BES) activities and on the NanoSummit that had been held in the spring.

Five themes have evolved in the strategic planning of BES: mission, science, tools, stewardship, and workforce. Over the years, BESAC has played a major role in meeting the mission challenges of BES, most recently through the publication of the Stringer-Horton report, *Basic Research Needs to Assure a Secure Energy Future*, and the follow-on study, *Basic Research Needs for the Hydrogen Economy*. Four subthemes have evolved among the challenges encountered in addressing BES's mission: the ultrasmall; the ultrafast; theory, modeling, and simulation; and complexity. BESAC has done a lot of work on the first two of these subthemes. A presentation will be made later in the meeting about the third. And BESAC has been heavily involved in the roadmap study on the fourth. In addition, BESAC has been involved in the 20-year facilities roadmap for the Office of Science (SC), and it continues to contribute to the development of the nanoscale-science research centers (NSRCs). Following on the Stringer-Horton report and the hydrogen report, the next BESAC workshop may very well be on Gen-IV fission and fusion energy in collaboration with other offices of the Department of Energy (DOE).

All five of these themes came together at the Secretary's NanoSummit, held on June 23-24, 2004. The meeting was a call to arms to use nanoscience to meet the nation's energy challenges. Rick Smalley gave a presentation at the NanoSummit that showed that 85% on the world's energy came from fossil fuels in 2003. Fifty years from now, the world will need twice that amount of energy, and most of it will have to come from sources that do not impact the environment. A seminal paper was published by Martin Hoffert et al. in *Nature* about future energy supplies being non-carbon dioxide producing. These studies underscore the need for BES to look at renewable energy resources. Another presentation at the NanoSummit by Nate Lewis underscored the great potential of solar energy. It pointed out that geothermal energy in North America has a total potential of 11.6 TW; technically feasible hydroelectric power could produce 1.6 TW; biomass from 50% of all cultivatable land could contribute 7 to 10 TW; wind, with 4% utilization, could generate 2 to 3 TW; and practical solar energy could produce 600 TW.

In response to these studies, the next BES workshop will address the following themes related to solar energy:

- Increasing the cost-competitive production of fuels and chemicals from renewable biomass by a factor of 100
- Developing methods for solar-energy conversion that result in decreasing the cost-to-efficiency ratio for the production of fuels and electricity by a factor of 0.10 to 0.02
- Converting solar energy into stored chemical fuels
- Developing advanced materials for renewable-energy applications

BESAC's input to this workshop was formally requested.

Separately, BES and BESAC have held a series of workshops to drive the development of BES's roadmap. These workshops have dealt with complex systems, nanoscale science, biomolecular materials, theory and modeling in nanoscience, catalysis, and theory and computing (currently under development). The question is what the next workshop should be. A workshop that addresses grand questions (e.g., as the National Academy of Sciences did in connecting quarks to the cosmos) may be needed. It might look beyond nano or complex systems or might look at the broad scheme of electron-volt science, which binds together disciplines that are connected by the common Hamiltonian. Chemistry and materials science are frequently relegated to "technology development," while excitement is heaped upon the new physics of dark energy, dark matter, etc. What is done in chemistry and materials science could have as equally dramatic an impact on the future as does the new physics. BESAC can capture some of these challenges, and Dehmer asked the members to determine how it could be done.

For the first time in 16 months, BES has a full complement of division directors. Harriet Kung is the director of the Materials Sciences and Engineering Division; Pedro Montano is the director of the Scientific User Facilities Division; and Walter Stevens is the director on the Chemical Sciences, Geosciences, and Biosciences Division. Two other positions have been filled, but there are still several vacancies in the organization chart.

At this point in time, FY04 is about closed. The FY05 budget is before Congress. DOE is providing guidance for the Office of Management and Budget (OMB) budget preparation for the FY06 budget. Planning for the FY07 budget request starts in March or April of 2005; the Office will need results from the workshops by that time to incorporate their findings into budgetary planning.

The FY05 President's budget request for BES is 5.2% more than the FY04 appropriation. The construction portion of that budget request is fairly large because of the activities related to the Spallation Neutron Source (SNS), the NSRCs, and the Linac Coherent Light Source (LCLS). The SNS construction is winding down, and the NSRC construction is ramping up. The amounts requested for the major budget categories are $231.9 million for construction, $178.3 million for university research, $240.1 million for national-laboratory research, $287.7 million for user facilities, and $81.8 million for capital equipment.

In the House, the committee recommendation for BES is $1,076,530,000, an increase of $13,000,000 over the budget request. The increase is to fund additional research on nanoscale science and increased operating time on the BES user facilities. The budget request is still awaiting action in the Senate and must then go to a conference committee.

A study of the Energy and Water Development appropriation bills that have been signed during the past 15 years shows that two-thirds of them have been signed after September 30th. That for FY03 was signed 143 days after the beginning of that fiscal year. In four of the past five years, the appropriation bills were signed well after the beginning of the fiscal year. Happily, Congress does not have metrics that they are graded on.

The BES web site has been upgraded.

A solicitation for research in support of the President's Hydrogen Fuel Initiative is under way. Approximately $21.5 million will be awarded in FY05, pending appropriations. (The House has approved the appropriation; the Senate has not yet acted.) Five high-priority research directions were the focus of the solicitation:

- Novel materials for hydrogen storage
- Membranes for separation, purification, and ion transport
- Design of catalysts at the nanoscale
- Solar hydrogen production
- Bioinspired materials and processes

No full applications will be accepted without a preapplication followed by a BES response encouraging a full application. Each federally funded research and development center was limited to the submission of six preapplications as a leading institution. Initial awards will be in FY05. BES will coordinate very closely with all appropriate groups, particularly the Office of Energy Efficiency and Renewable Energy. The first discussion of this solicitation at BESAC was on February 23, 2004. The call for preapplications was published May 15, 2004. Preapplications were due July 15, 2004. Decisions on preapplications will be sent to principal investigators (PIs) by September 1, 2004. Full proposals will be due January 1, 2005. Awards will be made in June or July 2005. More than 700 preapplications were received, and the qualified submissions are being reviewed by panels of federal employees. The distribution of qualified submissions was, storage: 199; membranes: 174; catalysts: 152; solar: 86; and bioinspired: 54. The proposals requested $250 million for the first year, a factor of 10 over the amount that is available.

The DOE program plan calls for BES to provide "world-class scientific research capacity needed to: ensure the success of Department missions in national and energy security; advance the frontiers of knowledge in physical sciences and areas of biological, medical, environmental, and computational sciences; or provide world-class research facilities for the nation's science enterprise." The BES Mission Statement and Program Goal has to relate to that program plan and its general goals. To ensure that it does, the OMB Program Assessment Rating Tool was created by this administration. The President's management agenda requires planning and reviews of that planning. It also requires long-term measures of performance. Expert review every three years will rate progress as "excellent," "minimally effective," or "insufficient."

BES's long-term measures of its materials-science activities call for it, by 2015, 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. *Success* is defined as follows: 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 follows: BES-supported research leads to a steady stream of outputs of good quality.

BES's long-term measures of its chemistry activities call for it, by 2015, to demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy-transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems. The Committee of Visitors (COV) has to determine how to measure this progress. This is an additional charge to and responsibility of the COVs.

BES's long-term measures of its transfer-to-technology activities call for it, by 2015, to develop new concepts and improve existing methods for solar-energy conversion and other major energy research needs identified in the 2003 BESAC workshop report, *Basic Research Needs to Assure a Secure Energy Future*.

BES's long-term measures of its facility and user activities call for it, by 2015, to demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Bucksbaum noted that the hydrogen-economy initiative is responding to the President's stated priorities, but the solar-energy initiative requires changing the administration's orientation. He asked if this has ever happened before. Dehmer responded that it had happened with the hydrogen initiative, which was greeted with hostility by the administration at first. The same challenge is being faced with the solar-energy initiative. The mindset has to be changed from a 10-year outlook to a 50-year outlook, and the impact of the program has to be re-recognized. There will also be a turnover in personnel in the government, no matter who wins the upcoming election.

Kohn made a series of observations. (1) He welcomed the Secretary's announcement of the creation of an Office of Science Education and said that he was thrilled with this major change. (2) The terminology of "string theory" was bad for science (and wrong). (3) He pointed out that complexity is *not* a field. Everything that is not trivial is complex. The term should not be used. (4) The CEO of Shell says that the threat of carbon dioxide is much greater than that of terrorism. Global warming *is* a serious problem. (5) The Stringer report is a few years old. The problems involved in making solar energy commercially promising have changed. Instead of 10 to 50 years to commercial viability for solar technology, society is probably 2 to 5 years from that point because of the advances that have been made in the past decade.

Richards pointed out that Nate Lewis had not talked about fission; moreover, he did not point out that the hydrogen must be obtained through the use of other fuels. The *real* problem is making new energy and storing it in hydrogen. Dehmer observed that this gets to the difference between the approaches of the Technology Office and BES.

Cummings asked if the BES solar report and the BESAC visionary report that she mentioned were two distinct reports. Dehmer replied, yes. Cummings went on to ask if she wanted BESAC to conduct the visionary workshop. Dehmer answered that, if BESAC could do that, it would have a big impact. Rarely do discipline-oriented reports provide any surprises. It is time to initiate a discussion on future grand challenges for the fields overseen by BES. Hemminger commented that conducting such a workshop would require one to define *how* to think about these topics, not just holding a workshop.

Moskovits noted that the NanoSummit was striking. The Secretary addressed many topics that were controversial. He asked Dehmer if she wanted BESAC to link up down-to-earth energy problems the way dark energy has called attention to experimental challenges. Dehmer said that she would not tie it to *just* energy. There are many questions that could be raised in the electron-volt region.

Stupp asked if her intent was to affect the planning of the 2007 budget and noted that this task requires tapping a broad community. Dehmer said that she would not link it too closely to the FY07 budget; one would not come up with the right answer. Hemminger commented that this workshop should be a driver of the scientific community, not of the budget.

McCurdy noted that some of NASA's projects have had no science content, and they now must identify science goals. He asked Dehmer if she were asking the committee to do a similar task. Dehmer responded that the National Academy of Sciences' *Connecting Quarks with the Cosmos* had other drivers. There is a perception that there are no grand challenges in chemistry and materials science. Some grand, unifying goal is needed. As a community, chemistry and materials science should think in a grander way.

Bucksbaum stated that BES has a lot to do with the future success of investigating global warming and dark matter. The community needs to think of what is beyond those catch phrases, a real challenge that has not been on the agenda before.

Isaacs asked how unbounded the workshop should be in considering problems. Dehmer replied that it has to give the committee an actionable charge. Hemminger stated that the areas are broadly constructed (electron-volt science).

Flynn said that one should distinguish between (1) a thrust area (e.g., the hydrogen economy), where technology has evolved to a point where old ideas can be effectively re-addressed, and (2) a grand challenge.

Moskovits said that he would like to put forward six potential topics: the early steps in DNA-based life, nonreductionist approaches to systems, the concept of reversibility, string theory, highly turbulent systems, and recycling. [A nonreductionist approach would not dissect a frog to determine its component parts but would, rather, ask the question, "What is frogness?"]

Williams added the topics of photonics and thinking about light as a quantum-mechanical phenomenon. Opportunities are arising (e.g., Piper-Raman scattering and photon entanglement) at the leading edge of understanding the universe. In looking at the quantum-mechanical basis of electromagnetic radiation, there will be more changes in this area in the next decade than there have been to date. It will encompass chemistry, materials science, laser facilities, etc.

Cummings noted that the systems approach is emerging in many disciplines. It is another word for complexity.

Stupp said that one problem is the notion of creating permutations of things. That is how science is evolving. This is a disease state. One does not make quantum leaps this way. One cannot scale up or prototype something with a function. Many phenomena have not been discovered because the macroscopic prototypes have not been made. High-energy physics is different. From chemistry, people expect something *useful*. Chemistry and materials science have this problem. It is worth thinking about the translational aspects of the advances that have been made in the past decades.

Flynn said that imaging from atoms to animals is a technology that is coming together and is a great thrust area.

Hemminger said that the Committee needs to think functionally about how one conducts such a workshop. He hoped to continue this discussion the following day. He declared a break at 10:27 a.m.

The meeting was called back into session at 11:08 a.m. to receive the report of the User Facilities Division Committee of Visitors (COV). Hemminger pointed out that the new uses of these COV reports by OMB will stress the COVs by requiring them to provide advice to OMB; he hoped that this would not prevent COVs from conducting a candid analysis of what is going on. He introduced **J. Michael Rowe** to present the User Facilities Division COV report.

Rowe said that the COV members had lengthy discussions with the BES Science Advisory Council, which were quite helpful. He identified the members of the COV.

The charge to the Committee was (1) to assess the efficacy and quality of the *processes* used to solicit, review, recommend, and document actions leading to the upgrade or construction of facilities or to special research activities related to facilities, such as detector development or accelerator physics [the Committee did not do much of this; there was not much of a record to look at in terms of solicitations], (2) to monitor operating facilities, and (3) to comment on how this review process has affected the national and international standing of the individual facilities and the collection of facilities operated by BES.

The Committee broadened the charge immediately because this is a new division, still developing policies and procedures, and because the scale of projects is quite different from the other two divisions. The peer-review process is, of necessity, different from that for PI grant processes. The Committee chose to interpret the charge broadly and to focus on the establishment of the new Division and issues relating to the review process itself.

A two-day meeting was held in Germantown with presentations by Pat Dehmer and Pedro Montano. Three groups looked at the history for the three major types of facilities (neutron, synchrotron, and nanoscience facilities), with individual cross-checking with other groups. Extensive executive sessions critiqued document availability.

The COV also sent letters to each BES facility asking for comments. All agreed that the review process was fair and all said it helped; but there was not universal enthusiasm for the "assistance" rendered. There was no concern expressed about the need for metrics, but there was about the definition of metrics. Metrics are good, but need careful thought to make sure that they measure what is needed to be known. Facilities should be partners in developing metrics to make sure the metrics are applied uniformly from institution to institution.

In a review, the reviewers all listen to and read the same information but provide individual assessments. A concern was expressed about anecdotes becoming data without the checks and balances of consensus building. There is an appearance of the potential for bias. A lack of consensus *could* lead to ill-considered statements and recommendations.

Several issues were uncovered by the COV: It was not clear what had gone on in the past; there is a need for better documentation of prior assessments, including the recommendations and responses; these prior critiques and documents related to the responses they elicited should be included in the COV package. Currently, the Committee cannot tell if re-reviews were conducted. Cross-references to earlier reviews would help the COV better grasp the full history.

The necessary elements of the documentation of facility reviews include

- An executive summary that accurately and succinctly reflects the tone and substance of the review; letter responses to reviews to facility and laboratory management;
- Reporting of review outcomes to reviewers, and feedback on summary, recommendations, etc. (not currently shared with COV members);
- Care in informing reviewers of procedures and assuring them that the COV will have access in future [a quality-assurance issue; a lot of time is spent explaining the Federal Advisory Committee Act (FACA) procedures to participants]; and
- Re-reviews should be scheduled in cases where the normal schedule is too "leisurely."

The Committee considered success to be defined as

Success = Happy Users + World-Class Science

User needs are changing because how science is done is changing, and definitions must follow (e.g., mail-in samples, remote operation, and nanocenters). One must derive acceptable definitions of users, publications, and acknowledgements when only a (small) part of the research depends on the facility. One must also determine how the facilities affected the science that resulted from the research. Nano centers will accelerate these trends.

What metrics should be used? The COV approves of the use of well-defined metrics in evaluating facilities, with the caveats that a countable item may not be a good metric, terms must be clearly defined, metrics for neutron and photon facilities may be different from those for nano centers, and all metrics should be reviewed regularly in direct consultation with facility managers.

The COV concluded that reviews are fair and are seen to be so, but there is unease about individual reports, which may give inordinate weight to minor points and rely on the perceptions of outsiders and facilities. The COV review and its allowance for adequate facility responses help alleviate these concerns.

The COV offered the following suggestions for improvement:

- The definition and choice of metrics should be improved.
- User surveys on satisfaction should be required (by user groups).
- The division has to take strong control of the agenda to allow more executive discussion.
- Time should always be provided for direct reviewer contact with users and staff.
- When serious deficiencies are identified, a re-review should be conducted in a short time in addition to written responses.
- Time for discussion of laboratory-wide issues should be included (all of these facilities are embedded in larger institutions).
- Research program representation should be ensured at reviews.

It also offered the following recommendations concerning the operation of the NSRCs:

- Require intercenter collaboration. (Make different centers work with together.)
- Closely involve users at the beginning.
- Establish appropriate agreements with other laboratory activities and facilities.
- Coordinate between laboratories to ensure a national, not regional, resource.
- Carefully integrate the operations of the NSRCs with science programs.

The new structure of BES and the Facilities Division is good for all involved. It relieves science program managers from the details of facility operation. It allows research program managers to focus on *science* rather than the facility. It allows facilities to receive proper management attention, commensurate with their budget and impact. And, to some degree, it reduces the scope for budgetary arguments.

Why have we gotten around to this only now? There are actual and potential negatives in separating facilities from science. There is a loss of the sense that facilities serve science. Facility management is decoupled from research programs. It produces enhanced visibility (for good or ill). Because of all of these reasons, the COV recommended that both research divisions have at least one program manager at every facility review. The three divisions have to talk and work together.

In summary, the COV concluded that the new Scientific User Facilities Division is well launched, building on past facility management. The COV strongly supports the new structure. The facility reviews are working, although the COV recommended some changes and improvements. The COV strongly supports the NSRCs and recommends additional national planning and cooperation, making them an integrated national resource, not a series of regional resources.

Hemminger thanked the Committee.

Kohn noted that he preferred the equation

Success = Great Science + Happy Users

Rowe agreed to the change. Kohn asked how the executive session worked. Rowe replied that one can discuss issues but not collaborate in the writing of the final report. Each reviewer prepares a separate report, which is then synthesized with all the other reports, as required by law.

Gates asked to what degree the ultimate source of information was the users themselves. Rowe responded that the information comes from the files, the extant record. There will be users present; the COV solicits their comments. They should submit their own report to the COV.

Richards liked the idea of making the NSRCs cooperate. The COV report stresses the need for institutional memory. Such memory requires that the information be written down. At the same time, some information is given to the facilities orally. He asked how the Committee reconciled this. Rowe said that it is all included in the final report; the oral presentations are just more detailed.

Berrah noted that the NSRCs will be different from the light sources, so the COV should come up with a mechanism to assess users' experiences at different centers.

Bucksbaum asked whether the User Facilities Division can assess when a facility has outlived its usefulness. Rowe responded that these reviews are designed to assess if the facility is producing good science, which is part of that question. Other types of reviews (e.g., multifacility reviews, comparing the different facilities) could also be conducted. This Division will likely improve this situation.

Williams asked whether there are formalized rules of engagement set up to see how the operators and scientists interact. Rowe replied that this is a concern that the COV had. No procedures are written down. The three division directors said that they do interact, but there is no formal structure. Dehmer said that the three division directors and higher management meet once a week informally. Representatives of the two other divisions will be present at all facility reviews. A meeting of all facility directors will be held to discuss metrics.

Johnson asked if there were procedures to prevent anecdotal information from being considered hard data. Rowe said that, if an individual reviewer reports an anecdote as data, the review process at the division level is relied upon to edit it out. The issue had been raised because people are sensitive to it.

Hemminger noted that the COV had expressed that it would be useful to have a more formal assessment of the Division's responses to prior COV recommendations and he asked if representatives should be required to come back to BESAC and detail how they responded to the recommendations. Rowe said that the reviewers are not happy with being left in the dark about how their assessment turned out or about the responses to the recommendations. Dehmer commented that this is not unlike all peer-reviewer processes. She would (and has) reported on how BES has responded to the recommendations. There may need to be a review of the peer-review process. Rowe stated that he approved of the process.

Hemminger asked for a motion to accept the COV's report. Berrah moved, and Long seconded. The motion was approved unanimously. Hemminger thanked the chair and members of the Committee for their services and declared a break for lunch at 12:07 p.m.

Thursday, August 5, 2004
Afternoon Session

The meeting was called back into session at 1:37 p.m. Hemminger said that the next COV would review the Chemical Sciences, Geosciences, and Biosciences Division in mid-April 2005. Gordon Brown will chair that COV. Hemminger asked the Subcommittee on Theory and Computation to provide an interim report on its activities. A final report is due in the fall. **Kate Kirby** was the first of three presenters of that interim report.

The charge to the Subcommittee is to identify current and emerging challenges and opportunities for theoretical research within the scientific mission of BES, with particular attention paid 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 and to guarantee that BES researchers will be able to exploit the entire spectrum of computational tools, including the leadership-class facilities contemplated by SC.

A planning meeting of the Subcommittee was held February 22, 2004. On April 17-18, 2004, the Subcommittee met in Chicago to take testimony from selected members of the community. It then prepared a letter report to John Hemminger and Pat Dehmer for discussion at this meeting of BESAC. On July 30, a first draft of an extended outline was delivered to the entire Subcommittee. Responses and input are being awaited. Another meeting will be held in the fall, and the proposed final draft of the full report will be delivered to BESAC for its evaluation at its December meeting. The final bound report will be delivered to SC and the Subcommittee members at the end of January 2005.

Kirby reviewed the membership of the Subcommittee and displayed the working outline of the report.

Why invest now in theory and computation? There is a confluence of events that have transformed theory and computation:

- The striking recent scientific successes of theory and modeling;
- The appearance of many new scientific frontiers;
- The development and construction of new experimental facilities; and
- The ongoing increase of computational capability, including the promise of a new leadership-scale computational facility.

Examples of the dramatic progress in theory and computation include:

- Density functional theory (DFT) has transformed theoretical chemistry and surface and materials science.
- Large-scale classical molecular dynamics has been able to treat the motion of more than a million atoms.
- Discrete grid and wave-packet methods have been developed for treating atoms/molecules (e.g., in intense fields).
- A range of electronic structure methods have evolved, such as coupled cluster, many-body perturbation theory, and quantum Monte Carlo.
- First-principles spin dynamics elucidated the mechanism of giant magnetoresistance and spintronic devices.
- Dynamical mean field theory (DMFT) has been successful in describing strongly correlated electronic states that had not been amenable to analysis.

- Ab initio molecular dynamics (Car-Parinello) treats motion of atoms and changes in electronic structure during that motion.

As a result of these advances, many new scientific frontiers have evolved through innovative experiments. They have raised great challenges to theory. These new frontiers include nanoscience, ultrafast chemistry and physics, biomaterials and biomimetic systems, coherent control, control of quantum coherence, and spintronics.

At the same time, new experimental facilities have emerged. Existing light sources [e.g., the Advanced Photon Source (APS at Argonne National Laboratory), Advanced Light Source [ALS at Lawrence Berkeley National Laboratory (LBNL)], and the National Synchrotron Light Source [NSLS at Brookhaven National Laboratory BNL)] together with the new LCLS under construction [at the Stanford Linear Accelerator Center (SLAC)] have created a growing wave of new experiments in chemistry, physics, and materials science. Completion of the construction of the SNS at Oak Ridge National Laboratory (ORNL) is scheduled in 2006. Five NSRCs are under design or construction. What is needed is an overall strategy and increased support for theoretical research to guide and respond to the amazing array of experiments at these facilities.

New computational capabilities have also become available. Desktop workstations have seen a rapid growth in microprocessor speed (Moore's Law). Cluster computing (tens or hundreds of processors linked together and run by a single research group or department) have helped to ready many disciplines within BES for massively parallel computing. Large-scale computing facilities operated by DOE, the National Science Foundation (NSF), and others are being used for BES research in all these areas at centers at the National Energy Research Scientific Computing Center (NERSC at LBNL), ORNL, and Argonne; a new facility at Pacific Northwest National Laboratory (PNNL) and a leadership-class facility at ORNL are under development. There is a need for the right computational capabilities across the spectrum.

The open meeting in Chicago featured more than 16 invited talks plus panel discussions. A website was established to collect input. E-mails were invited to the website or directly to the co-chairs. An announcement inviting input was posted on the American Chemical Society Division of Physical Chemistry home page. In summary, the questions asked were:

- In your field, what are the major scientific challenges?
- In your area, do theory and computational science drive progress and/or partner with experiment?
- How might progress in your field impact other areas within BES?
- Are computing resources (hardware and software) a limiting factor in your field?
- Would support for development of new algorithms for high-end computer architectures be important?
- Are there opportunities in your area to assemble interdisciplinary teams for attacking large problems?

On the website, 44 scientists responded to this request. An important consensus observation that emerged was that theory and computation should be viewed as a unity, not as competing parts of the BES portfolio. The theory enterprise in BES is extremely heterogeneous with respect to the scientific problems, the research group size, and the computational resources required. Ensuring the highest quality scientific return requires the complete spectrum of theory.

Kirby turned the floor over to **William McCurdy**, who noted that Dehmer had asked for two or three areas of theory that could be used in forming a roadmap for BES science. The subcommittee found that BES has an immensely diverse portfolio, which is one of BES's greatest strengths.

The original working list of 25 specific opportunities contained about 15 areas and outstanding problems, and this list was reduced to 8 in discussions and votes of the subcommittee. Several important areas of the BES portfolio were not represented in the initial verbal testimony, but some of those are addressed by written testimony. These eight may not be the final list that appears in the full report. The Subcommittee tried to organize these areas into themes.

Complexity and control are already well-established themes of the BES portfolio. The Subcommittee divided complex systems into (1) quantum control of physical systems and (2) control of complex systems. The topics that floated to the top were

- Nanoscale materials (which is too broad a topic) and phenomena;
- Correlated electrons in solids (the whole collection of phenomena), such as high-Tc superconductivity; colossal magneto-resistance; and exotic magnetic phases, correlating electron motion with atomic motion;
- Excited electronic states, which is still the holy grail of electronic structure; many aspects of which have not been addressed;
- Defects in solids, the Ur problem for bridging the atomic and mesoscopic length scales to understand strength, transport, fatigue, and magnetic hysteresis;
- Quantum control of physical systems, which encompasses two notions, quantum control (e.g., of chemical reactions by shaped pulses of energy) and quantum coherence;
- Ultrafast physics, which is largely driven by new experimental facilities (as the attosecond regime is entered, this technique will determine if the excited-electron-state problem can be solved);
- Magnetic-spin systems and single electron devices that exploit the processes on spin transport and electron transport; and
- Understanding photochemical and enzymatic processes leading to improved charge-transport mechanisms and ultimately to engineering-level control of biomimetic energy production and self-assembly.

Catalysis is not included in the list. It is obviously important to DOE, and it has a large overlap with nanoscience. McCurdy was surprised that little testimony was offered on catalysis and speculated that the omission was a factor of the Subcommittee's sampling.

Other topics that did not make the cut included:

- Heavy-element chemistry, especially relativistic treatments;
- Turbulent reacting flow in combustion and granular flow; and
- Photonic materials and optical control at the micron scale.

The Subcommittee could not come in with 25 topics. However, it is not clear that the discussion has converged on what this Committee will be happy with.

McCurdy turned the floor over to **Bruce Harmon**.

Advances in underlying methods drive expansion in many other disciplines. For example, biologists are excited about changes in materials science (e.g., membranes). The Subcommittee considered whether there is a connection of the theory program with the BES facilities.

The APS, ALS, National Synchrotron Light Source (NSLS), Intense Pulsed Neutron Source (IPNS), Los Alamos Neutron Science Center (LANSCE), and High-Flux Isotope Reactor (HFIR) all have little or no associated theory program. Users must find theoretical collaborators to work on their problems who are willing and already funded. (This is the Blanche DuBois method: depending on the kindness of strangers.) There is a need for stronger coupling of theory and computation with experiments at BES facilities.

New major experimental facilities are pushing the need for theory. There should be coordination among the theory sections of the five nanoscience facilities, the SNS, and the LCLS. What is needed are (1) motivation to integrate theory partnership in the planning stages to accelerate discoveries and (2) understanding and to enhance the efficacy of these facilities.

The integration of the theory program with the BES facilities will enhance scientific productivity. In a mature area, it will produce interpretation of experiments (allowing meaningful pursuit of more complex systems). Without the theory component, experimentalists would not understand their data. Without theory, one does not know what one is looking at. In an emerging area, theory will suggest new areas of inquiry and propose new kinds of experiments.

A number of mode-coupling issues exist: Should theory capabilities be in-house or distributed? There have been good examples of both. Should they support directed research and/or blue sky research? Should they serve collaborative research teams and/or single PIs? Collaborative research teams are designed to advance frontiers in computational materials science by assembling diverse sets of researchers committed to working together to solve outstanding problems that require cooperation across organizational and disciplinary boundaries. For example, a team investigating excited-state electronic structure has been operating for 5 years, producing new ideas, theories, computational methods, and codes that are passed on to the community.

Resources are a big issue. There must be a unity of theory and computation. A hierarchy of computational resources is necessary to express modern theory with leadership-scale capability; high-performance, massively parallel, large-scale capacity; and local computing resources (e.g., clusters). Scientists need to be able to look at thousands and hundreds of thousands of atoms simultaneously. One cannot distribute the computing; there has to be a base of programs and people that understand them. One million node-hours on a supercomputer can be matched by a 60-node cluster. Clusters are on the market a month after a faster CPU comes out.

There is a need to keep people in the theoretical activities. Support must be provided for long-term software projects, building the community codes as infrastructure for theory and experiment. European programs have set an example. The VASP/WIEN Project in Vienna came from BES’s Dale Koelling; Vienna puts up $300,000 a year to maintain it. Another example is NIH’s funding of Klaus Shulten’s work on NAMD molecular-dynamics code at the University of Illinois. The development of robust software helps a lot of communities. The question comes down to whether there should be a renewal and expansion of the SciDAC style of large-scale project support in BES. Only the Chemical Sciences Division participated in SciDAC and only at a level of $2 million/year. Besides funding, there is also the problem of getting the necessary teams together.

A lot of money is being put into new facilities, instruments, and supercomputers. These virtual user centers have not been well thought out but do have open-source repositories, object-oriented tool kits, workshops, and education programs. However, they are underutilized and need to mature.

As an example of why the Subcommittee was so excited about this topic, Harmon noted that his dissertation work took 9000 hours on a supercomputer. Today the whole project can be done in 26 seconds on his desktop.

Stupp asked what the status of biomimetics was. McCurdy said that it was a part of another discussion; no one at the workshop spoke about biomaterials. Stupp was surprised that it was not featured more. How molecular components organize is an important question. Theory needs to be employed here. Even in electronic structure, molecular organization is important and interesting. Another example is that ordinary ground-state molecules are being discovered to be catalysts. Stupp said that he would like to see a roadmap for outreach to the research community, telling experimentalists what theorists can do for them. He said that he had to educate himself on how to interact with theorists. That skill is not taught in schools.

Williams noted that theorists must also be educated about what experimentalists are all about. His experience was that brilliant theorists turned into inventors. They bring to the table a new set of tools and expertise and an “unfair” advantage. The organizational principal employed here could have been themes. A matrix approach might help optimize the selection of areas to be addressed. One could look to see if any cross-cutting approaches have footprints in several cells of the matrix. Tremendous computational capabilities are now available, and one might be able to use a brute-force approach effectively, at least at first. Kohn said that he had heard of that type of work being done at the National Renewable Energy Laboratory by Alex Zunger. Zunger has the concept of describing a function and computing a structure that would produce that function.

Cummings said that some of the things that Stupp cited will be in the nanoscience part of the report. Catalysis probably did not emerge because of the mix of contributors; it will probably be incorporated into the report.

Clark asked if catalysis is on the list or not. McCurdy replied that it is not now on the list, but the Subcommittee is seeking more input. Clark asked if the relativistic treatment of heavy-element chemistry is separate. McCurdy answered that it was proposed to be one of the final eight but did not make the cut. Clark observed that it is such a small community, one might easily miss it.

Berrah commented that retaining young theorists is also an important issue that could be addressed. Theory is not funded. The young theorists must be nurtured.

Bucksbaum offered a different organizational principal for finding commonality: themes of problem solving. The molecule knows how to solve Schroedinger’s Equation faster than the computer does. A “virtual instrument” would put researchers in a new league, and BES could build a bridge there.

Long observed that researchers are constantly going back and forth between experiment and theory, and they appreciate the efforts available from the full spectrum of capability.

Plummer worried about what this does to the ingenuity of the creative mind. One does not want to turn off the phenomenological theorists. Brick-and-mortar theorists are needed at the facilities. However, there cannot be just 1/100th of a theorist at the other end of a telephone line. A researcher needs to walk down the hall and sit down and talk with a real person.

Moskovits noted that this group had touched on a number of resonant topics. He would have liked to have seen the full list of 25 ideas. Some may be ideas before their time. It would be great to have another study on inherent intelligence. Real mathematicians should be included. Interaction of mathematics and physics is now done at the real-life level.

Isaacs said that, in the end, it is the postdoc walking down the hall to talk to a theorist that makes a difference, localized software notwithstanding. It is crucial to have the grand challenges identified.

Johnson pointed again to the three areas that surprised McCurdy by not getting into the final eight. That some of these did not make the final list means that more effort needs to be put into the winnowing down of the list.

Kohn made several observations. (1) A conceptual theorist is necessary to supplement the transparency infrastructure referred to by Harmon. A conceptual theorist can have an important impact. (2) The light source at LBNL has an advisory committee with *no* theorist among its 35 members. (3) When one deals with excited states, one gets into a new era of combinations of high intensities and high frequencies, and it is a new ballgame in these regimes. (4) Moore’s Law is flat in comparison to conventional quantum chemistry. DFT scales linearly. Electronic nearsightedness makes complex situations much simpler. That is the physical basis of mathematical scaling. If Moore’s Law becomes real, quantum computing will extend our capabilities from 10,000 atoms to millions. Even if it is not realizable, it will pose so many important questions that pursuing this dream is prudent.

Gates said that the way the list of eight or nine topics is formulated puts less emphasis on chemical topics. If a different notational system were used, a lot of issues could be lumped together and included.

McCurdy noted that many people had spoken to Plummer’s concern about the loss of creativity. Computing cannot replace the human mind. The charge focused on high-end computing. The progression had been from conceptual to computational theory. The conceptual regime must be revisited in this report. A whole collection of mathematicians, computational chemists, theorists, etc. are needed. To paraphrase a common saying, it takes a *village* to raise a theory.

A break was declared at 3:30 p.m. The Committee was called back into session at 4:00 p.m. **Mary-Anne Scott** of the Office of Advanced Scientific Computing (ASCR) was introduced to present an update on the Energy Sciences Network (ESnet). ASCR provides interoperable computing infrastructure to DOE researchers.

ESnet’s mission is to provide interoperable, effective, and reliable communication infrastructure and leading-edge network services that support DOE missions, especially those of SC. It enables thousands of DOE, university, and industry scientists and collaborators worldwide to make effective use of unique DOE research facilities and computing resources independent of time and geographic location. It provides direct connections to all major DOE sites and access to the global Internet (managing 150,000 routes at 10 commercial peering points). User demand has grown by a factor of more than 10,000 since its inception in the mid 1990s, a 100% increase every year since 1990. It provides capabilities not available through commercial networks. It is architected to move huge amounts of data among a small number of sites and to provide access to U.S., European, Asian-Pacific, and other research and education networks with high-bandwidth peering.

ESnet is a community endeavor. It receives strategic guidance from the SC programs through the Energy Science Steering Committee (ESSC). Network operation is also a shared activity with the community through the ESnet Site Coordinators Committee, which ensures the right operational "sociology" for success.

The current vision for ESnet has evolved from a series of workshops that called for a scalable, secure, integrated network environment for ultrascale distributed science to make it possible to combine resources and expertise to address complex questions that no single institution could manage alone. A workshop was conducted on network strategy and came up with a production network that provides (1) base TCP/IP services that are +99.9% reliable; (2) a high-impact network that offers increments of 10 Gbps and switched lambdas that are 99% reliable; and (3) a very flexible research network (UltraScience Net) that interfaces with production, high-impact, and other research networks and starts the advance toward optical switching.

The network's management has also revisited the governance model to incorporate SC-wide coordination and advisory-committee involvement.

BES and its researchers contribute to the planning through (1) early identification of requirements in terms of evolving programs and new facilities, (2) participation in management activities, and (3) interaction with BES representatives on the ESSC. The next ESSC meeting will be Oct. 13-15 in the Washington area.

She turned the floor over to **William Johnston**.

ESnet provides (1) a production network without which the national laboratories could not function and (2) UltraScience Net for large-scale data transport. It tries to provide full access to the global Internet for DOE laboratories and comprehensive user support. It also provides a set of Grid middleware and collaboration services supporting collaborative science.

Essentially all of the national data traffic supporting U.S. science is carried by two networks, ESnet and Internet-2/Abilene (which plays a similar role for the university community) and is handed off in the international arena. There are a lot of local networks run by universities and others.

When a user sends a message, the first thing that happens is that the domain name system (DNS) retrieves a 32-bit address. The message and this address are sent to a router, which moves data in a hot-potato manner to a gateway router at the periphery of the local site. That gateway router implements separate site and network provider policies (including firewall policy). The message then goes on to a border router, which sends it on to a core router with (1) cybersecurity policy and (2) addressing of peering policy. The message moves through the core network until it reaches the appropriate exit core router, which kicks it out to a series of peering routers that lead it to the router of a big Internet service provider (ISP). The ISP will kick the message out to a router near the final destination and ultimately to the gateway router on that destination. The message will wend its way through a series of routers at that site until it arrives at the server for which it was intended. Along the way, electric channels might be converted to lambda channels so the message can be carried on an optical fiber network before being converted back into electrical channels at the end of its journey.

ESnet is a large data-communication ring that passes through hubs in the Bay Area in California, Chicago, New York, Atlanta, and El Paso before returning to the Bay Area. Many other links, loops, and networks are connected to it along the way as well as four high-speed peering points for transmissions to other large-scale networks in the United States, Europe, and Asia. ESnet is a Tier 1 router connected to virtually every other peering point on the Internet. Peering points exchange routing information that allows each router to determine which packets it can get closer to their final destinations. There is no set route from one point to another on the Internet. At the same time, peering is not random. Each decision along the route is made according to a logic that discriminates among available routes based on their proximity to the final destination of the packet of information being handled. This method of routing messages produces a massive number of potential routes. As a result, when users want to get to someplace out of the ordinary, they can get there, usually in a matter of milliseconds.

It takes several years to make changes in a network like this. A workshop was held to consider usage by seven major DOE science disciplines: climate, SNS neutron science, macromolecular crystallography, high-energy physics (HEP), magnetic fusion energy, chemical sciences, and bioinformatics. These disciplines can be clustered into (1) long-term data; (2) "control loop" data analysis; and (3) distributed, multidisciplinary simulation. Each discipline's near-, mid-, and long-term needs were analyzed. For example, in the next few years, climate research will need primarily a few data repositories and many distributed computing sites. In 5 years, it will need to distribute large chunks of data to major users for postsimulation analysis. In 5 to 10 years, it will need distributed, multidisciplinary simulation. Of interest was the throughput capabilities that each discipline would need in 5 to 10 years. All of these disciplines have about the same needs: a throughput of $n \times 1000$ Gbps and (in some cases) QoS [quality of service] for the control channel.

The predictions of 2 years ago (a 100% per year increase in traffic) have come true and continue. Annual growth in the past 5 years has increased from a factor of 1.7 per year to just over a factor of 2.0 per year. ESnet is currently transporting about 250 terabytes per month. The traffic rate is not transient; daily and weekly averages are about the same. SLAC is by far the largest user of ESnet, sending 1.5 terabytes per day to France, Italy, and Germany and accounting for more than 50% of ESnet's total traffic.

ESnet is a critical part of the large-scale science infrastructure of HEP experiments today. As other large-scale facilities (such as the SNS) come online, this fact will be true across DOE. ESnet is a visible and critical piece of the DOE science infrastructure. If ESnet fails, tens of thousands of DOE and university users know it within minutes, if not seconds. Therefore, ESnet has to have high reliability and high operational security in its network operations and infrastructure support, including automated, real-time monitoring of traffic levels and operating state of some 4400 network entities in the primary network. The core of the network is its routers, which are totally redundant. Engineers are located at four locations (Silicon Valley, LBNL , Ames National Laboratory, and BNL). The core operations in Berkeley will soon be replicated at BNL. Each location has two weeks of diesel fuel to keep everything running in case of emergency.

Thirty minutes after the Sapphire/Slammer worm was released, 75,000 hosts running Microsoft's SQL server were infected. Today, that infection would be shut down in 25 seconds. ESnet can damp out such a large-scale attack quite quickly, now. At each laboratory, a filter is put on incoming traffic at its ESnet gateway router (and outbound traffic, too). Filters on ESnet's border routers assist a site in coping with such an attack. Filters are also in place on the ESnet ring as a first line of defense. ESnet's second-line response is to filter traffic from outside of ESnet. Its third response is to shut down the main peering paths and to provide only limited bandwidth paths for specific "lifeline" services.

The main workers in the ESnet ring are the racks of equipment that hold the routers, interfaces, data and control exchanges (DCXs), power converters, and secure servers. Such a rack in a network hub costs almost $2 million.

ESnet uses X.509 identity certificates and Public Key Infrastructure (PKI) to provide secure, cross-site authentication of people and systems. ESnet negotiates the cross-site, cross-organization, and international trust relationships to provide policies that are tailored to collaborative science in order to permit the sharing of computing and data resources and other Grid services. This service was the basis of the first routine sharing of HEP computing resources between the United States and Europe.

ESnet also offers voice, video, and data telecollaboration service as a convenience to the national laboratories.

ESnet was included in SC's Facilities of the Future report.

During the next 10 to 20 years, ESnet *must* provide (1) capable, scalable, and reliable production IP networking with an average reliability of 99.999%; (2) network support of high-impact science; and (3) "science services" to support Grids, collaboratories, etc.

The current core ring has good capacity and resiliency; no one break can shut down the traffic. However, in the future, ESnet will need higher bandwidth, QoS, network-resident cache-and-compute elements, and robust bandwidth (multiple paths).

ESnet's new architecture goals are

- To have fully redundant connectivity for every site and high-speed access for every site (at least 10 Gbps);
- To put all the national laboratories on metropolitan-area rings with two connections into every facility (which has already been done for San Francisco in New York City);
- To establish a subloop of the backbone (two links across the current loop) for Los Alamos National Laboratory (LANL), Sandia/Albuquerque, and ORNL;
- To connect all the metropolitan-area rings in ten years with a second ring (which will originally be done at 10 Gbps, scalable to 40 or 50 Gbps); and
- To provide a 40-Gbps connection to Europe out of Chicago.

In conclusion, ESnet is a critical infrastructure to DOE's science mission. It is focused on the SC national laboratories, but serves many other parts of DOE. It is essential for large-scale science. ESnet is working hard to meet the current and future networking needs of DOE mission science in several ways: by evolving a new, high-speed, high-reliability, leveraged architecture and by championing several new initiatives that will keep ESnet's contributions relevant to the needs of the community it serves.

Hemminger asked if the architecture to Europe and Asia is a loop, also. Johnston replied, yes, but not with the same bandwidth (10 gigabits per second on the ESnet vs. 40 to GEANT).

Bucksbaum asked to what extent redundancy is provided by other networks. Johnston noted that this is all commercial architecture provided by Qwest or their subcontractors.

ESnet has a redundancy through interconnects with Abilene, although the two networks serve different users. Others construct large networks like this (e.g., MasterCard and American Express). Big banks that exchange trillions of dollars a day have similar networks.

Cummings asked if the National LambdaRail was included in the diagram. Johnston replied, yes. It is a nonprofit corporation that will contract with many users. UltraScience Net uses one lambda on the National LambdaRail . ESnet may build a second loop out of the LambdaRail .

Williams asked if ESnet had close cooperation with CERN and others to work out architectures, protocols, etc. Johnston answer affirmatively. ESnet personnel get together regularly with representatives from the other United States, United Kingdom, Japanese, and European networks.

Isaacs asked if ESnet owned the metropolitan area network rings and rented the big loop. Johnston said, no. ESnet owns the local routers and builds its own network on the loop. It pays Qwest $4.5 million a year to maintain the network. The metropolitan area network rings are partnerships with other organizations (e.g., I-WIRE in Chicago). ESnet uses 1 out of ~5000 circuits in Qwest's $1.5 billion optical ring. ESnet will always maintain an IP quality service. To bring down the ring requires a dual-point failure, which is unlikely.

Hemminger called for public comment. Kohn asked Dehmer about the new science-education initiative. Dehmer said that it is new, and she did not know about the budget or program in the out years. It does not have a director. It will probably be housed in SC. It is supposed to be funded in FY05, but it is not included in the FY05 budget before Congress now. Previously, Congress had suggested that education was not DOE's mission, so the prior efforts were shut down, but every secretary has pushed for its reinstatement. Orbach has pushed very hard for it.

There being no other comments, Hemminger adjourned the meeting for the day at 4:55 p.m.

Friday, August 6, 2004

Hemminger called the meeting to order at 9:04 a.m. and reviewed the schedule of the rest of the meeting. He introduced **James Decker** to present an update on the Office of Science.

Decker thanked the committee members for their hard and important work.

The FY05 budget request has been acted on by the House but not by the Senate. The House added $169 million to SC's budget request. The distribution of those additions (and reductions) is

- ASCR $30 million was added to the budget, most of it for computer hardware;
- BER The President's budget was reduced $134 million from that of FY04; the House added $17 million [including $5 million for the Genome to Life (GTL) Facility] and $75 million in unspecified funding to be directed;
- HENP $16 million was added to the High-Energy Nuclear Physics budget, much of it for increased electricity costs at SLAC and for increased user time and improved user support at SLAC and Fermilab;

NP Nuclear Physics received an increase of $14 million over the request: $7 million for conceptual design work on the Rare Isotope Accelerator and $7 million for increased user time on NP facilities, such as the Continuous Electron Beam Accelerator Facility and the Relativistic Heavy-Ion Collider;

FES Fusion Energy Sciences received an increase of $12 million for increased facility run time, further work on inertial fusion technology and high-energy/density physics, and additional funding for the National Compact Stellarator Experiment.

The next step in the budget process is unknown; there may be a continuing resolution (or not).

In ASCR, the leadership-class computer award was made. DOE ran a competition among the SC laboratories. Four proposals were received (ORNL, BNL, LBNL, and SLAC), which were reviewed by outside reviewers. The proposal submitted by ORNL in partnership with ANL and PNNL was accepted. The partnership also includes three industry partners: IBM, Cray, and SGI. The facility will be used for DOE's mission-related research and by users from other agencies. How to use this machine is currently being considered. Access to the machine will probably be allocated to multidisciplinary teams and to the development of community codes.

Orbach has committed to producing a document on the future of the national laboratories, clarifying their contributions and responsibilities. This document grows out of the Facilities of the Future effort earlier this year. SC has some direction from Congress to produce 5-year plans for the national laboratories. This document will probably look out 20 years. It will be sort of a budget document with many uncertainties. It will be published this fall.

Decker pointed out that each national laboratory is operated by a contractor and is evaluated each year in two general areas: science and operations (financial management, safety, safeguards, and security). It has been decided to review and improve this process by

- clarifying why these evaluations are conducted (to improve performance and to support decisions to extend or compete these contracts),
- understanding the strengths and weaknesses of the process (these reviews have been pulled together by the site offices, and there have been some variations from site to site), and
- identifying performance incentives that should be in the laboratory contracts.

The Secretary's Laboratory Operations Board is also looking at some of these issues. A draft internal document has been completed; the final product will be issued in a couple of months.

Hemminger asked what the plans were for a DOE education initiative. Decker said that the Secretary announced at SLAC recently that teachers and students would be brought into the national laboratories to give them broader exposure to science. There is a science-education office in DOE; it is unclear how this will grow or be structured. There are science-education programs across the Department. SC will play a coordination role.

Kohn said that LLNL and LBNL are interested in an outreach program but have no budget. Decker replied that the Department has had such a responsibility since the early days of the Atomic Energy Commission. Congress cut those funds about 12 years ago. An effort is being made to build the activity back up.

Kohn noted that the NSF had tried to operate a supercomputing facility that was built top-down and flopped. Decker responded that SC is well aware of that history. It has been successful with NERSC and its predecessors. The NSF effort failed for many reasons. One was that those machines were sliced up to address small rather than large problems. Kohn noted that the NSF also established a number of mathematics institutes that flourished. Decker observed that they had been small efforts with little funding.

Kohn stated that the University of California operates three laboratories: Lawrence Livermore National Laboratory (LLNL), LBNL, and LANL. The contracts for all three of these laboratories are up for renewal. He asked to if there will be a separate review of the science at Livermore and Los Alamos and, if so, when that review will be available. Decker said that he did not know what the competition process would be, and the National Nuclear Security Administration (NNSA) runs its own evaluation process. Kohn said that the University has its own internal review process, but he found it to be totally useless. He asked if there was a *useful* appraisal of the institutions. Decker said that the contractors are free to run their own appraisals. His view was that SC's evaluations should be based on its own peer reviews, which are conducted on a 3-year cycle, sometimes more frequently. Kohn asked if those reviews were made public. Decker said, no. Kohn said that he believed that the regents of the University were unaware of those DOE reviews and rely solely on the internal reviews. Dehmer said that there is a record of the communication of the review results, which are sent to the laboratory management, not to the contractor. Hemminger stated that there are also program reviews that are communicated to the laboratory management. It is the *transfer* of those results to the contractor that is problematic.

McCurdy asked Decker and if he would comment on the Laboratories for the Future of Science. Specifically, is there to be advisory-committee input? Decker replied that Congress wants a DOE document. SC is sitting down with each national laboratory and is critically analyzing what the laboratories put on the table. There is probably not going to be any advisory-committee input.

Hemminger thanked Decker for his presentation. The next BESAC meeting is probably going to be the first week of December. He introduced **Altaf Carim** to present a summary of the activities of the NSRCs.

Construction of the NSRCs is progressing at the Center for Integrated Nanotechnologies (Sandia and Los Alamos), Center for Nanophase Materials Sciences (Oak Ridge), and Molecular Foundry (Berkeley). Ground was just broken for the Center for Nanoscale Materials (Argonne). A conceptual design is being developed for the Center for Functional Nanomaterials (BNL). Full operation should be attained in 2006 by the ORNL center; in 2007 by the LBNL, SNL/LANL, and ANL centers; and in 2008 by the BNL center.

Each of the centers has established a website. The brochure *Nanoscale Science, Engineering, and Technology in the Department of Energy* was updated in March. An NSRC Directors' Meeting and Stakeholder Discussion was held August 2-4, 2004. Several prior half- and full-day NSRC directors' meetings have been held from June 2002 to February 2004. These have been used to gather the center directors (and some others) to discuss common issues and to coordinate activities, such as website design, “jumpstart” user programs, user training, outreach, a BES nanoscience brochure, and workshops. In addition, there was an initial minireview of operating plans in February at which a comprehensive list of issues was raised that was added to at the subsequent directors’ meeting. These (primarily operational) issues were the primary basis for holding the extended Directors’ Meeting and Stakeholder Discussion just before this BESAC meeting. That meeting had about 75 participants, including the directors and several staff members from each NSRC, other scientific community stakeholders (members of NSRC scientific advisory committees, NSRC jumpstart users, etc.), BES management and staff, and representatives from other parts of DOE (Environment and Health and SC’s Environment, Health, and Safety).

In addition, each NSRC was designated to lead a half-day session, organize it, and take responsibility for the products of that session. The agenda included standardization among NSRCs; ethical, legal, social, and environmental/health issues; metrics for success of the NSRCs; theory, modeling, and simulation (a science-coordination topic); and coordination among NSRCs. In addition, there were two satellite meetings of project personnel on (1) conventional facilities and (2) environmental safety and health; these meetings were initiated by staff at the centers.

Issue papers were prepared for each half-day session of the main meeting, which contained discussion of several related areas. The outcomes of these discussions were 15 concise issue papers produced by the NSRC directors and staff. These documents serve as collective input on operational issues from the NSRCs. They will be the initial basis for development of DOE-BES issue papers. After consideration and revision by BES, the NSRCs will have another opportunity to comment before these issue papers are finalized and made more widely available. Some snippets of information from the issue papers are:

Review Criteria: The key criteria for evaluating the successful execution of this mission are high scientific impact, a productive and satisfied user community, and quality of user support. NSRCs should use the same criteria for success as the other BES facilities. Impact should be counted as the total output of both user science and NSRC scientific staff, but can be (and perhaps ought to be) articulated separately for the purposes of BES review and annual NSRC self evaluation.

Review Process and Documentation: The documentation should include an executive summary written by the facility in the form of a narrative that covers the overall scientific impact, effectiveness of the user program, and future vision for the facility. The list of recommended documentation included five categories, with considerable detail supplied for each: facility, instruments and laboratories, user access, impact, and future directions.

Intellectual Property: Full-cost recovery is required for proprietary research, and efforts should be made to secure appropriate intellectual-property control for proprietary users to permit them to exploit their experimental results. Standard practice is to have staff sign nondisclosure agreements, as needed. Also, standard, coinventions between a user and a staff member are jointly owned, according to the rules and processes of the host laboratory. Paul Gottlieb (DOE Assistant General Counsel for Technology Transfer and Intellectual Property) described the various options for working with users under currently existing DOE-approved processes. While existing approaches have many of the characteristics that the NSRCs would like to see, it did not appear that any of these approaches have all of the characteristics required to satisfy the needs of the NSRCs. Gottlieb encouraged the group to define the characteristics that it would like; he and others can help develop an approach to secure the proper authorities to operate in the desired mode.

Coordinated User Activities: A working group should be established to reach consensus about the uniformity of the NSRC user proposal. If it is agreed that a uniform format is desirable, this same group will design a uniform *proposal* format (not a central point of contact for all centers). To optimize inter-NSRC communication and minimize cost, it is recommended that each center exploit the video conferencing access grid. The frequency of meetings should be between 1 and 4 months or more frequently as the need arises. A committee should be formed to discuss coordination of user support (e.g., global access to all NSRCs and design/implementation of standard basic web-based training modules). A grid (or grids) should be designed of all equipment available across the NSRCs; it should be a standard item on each NSRC website. The utility and wide support for science-based events, such as the NanoSummit, should be expressed to DOE and other governmental entities. Coordination meetings may be held to make it easier to allow prospective users to decide which center(s) meet their needs best.

Hazard Control, Worker Safety, and Training: Experiments should undergo preexecution review and authorization for potential health, safety, and environmental considerations. An industrial hygienist intimately familiar with laboratory operations should be part of this review team and should sign off on the protocol. Nanomaterials should be handled using existing practices for materials of unknown and presumed toxic properties. Clear and documented practices for handling nanomaterials should be adopted. Where it is possible that operations involving nanostructures may cause airborne exposures, workers should wear personal protective equipment. Additional discussion on points of NSRC coordination in this area occurred at the satellite ES&H meeting.

A “grand challenge” workshop for the National Nanotechnology Initiative was held on March 16-18, 2004, sponsored by DOE-BES and by other National Nanotechnology Initiative (NNI) participating agencies via the National Nanotechnology Coordination Office. The report developed at that workshop was informed by other BESAC and DOE publications. It stated that energy conversion and storage is one of nine grand-challenge areas identified as part of the NNI since its inception in 2001. The flip side is that nanostructured materials were identified as a cross-cutting research theme in both the energy-security and hydrogen workshops. The workshop also produced an executive summary, nine research targets for energy needs, sidebars describing research targets and their energy impacts, and six cross-cutting themes that underpin the identified research targets. The nine research targets are

- Scalable methods to split water with sunlight for hydrogen production
- Highly selective catalysts for clean and energy-efficient manufacturing
- Harvesting of solar energy with 20% power efficiency and costs 100 times lower than the current cost of photovoltaics
- Solid-state lighting at 50% of the present power consumption
- Super-strong, light-weight materials to improve efficiency of cars, airplanes, etc.
- Reversible hydrogen-storage materials operating at ambient temperatures
- Low-loss power transmission lines

- Low-cost fuel cells, batteries, thermoelectrics, and ultracapacitors built from nanostructured materials
- Materials synthesis and energy harvesting based on nanobiotechnology

He cited two sample research targets: (1) nanostructured photovoltaics with the potential to result in cost, durability, and efficiency breakthroughs and with bandgap tuning, nanoscale structuring, and combinations of tailored nanoscale components that could facilitate broad spectral absorption and (2) solid-state lighting with semiconductor nanocrystals (quantum dots) and other nanoscale advances that could provide lighting with much-reduced power consumption. A 50% reduction in the total electricity consumed for lighting would save 4×10^{11} kW-h/year.

The workshop also identified six cross-cutting themes:

- Catalysis by nanoscale materials
- Using interfaces to manipulate energy carriers
- Linking all of structure and function at the nanoscale
- Assembly and architecture at the nanoscale
- Theory, modeling, and simulation for energy
- Scalable synthesis methods

This workshop was one of a series of “grand challenge area” workshops sponsored during the past 2 years or so by the NNI interagency group and/or individual agencies. There will be an overarching workshop next month to synthesize the outputs of these more narrowly focused meetings, identify gaps, and consider other aspects of the future of the initiative. This overarching workshop is in some senses a successor to the 1999 interagency Nanotechnology Research Directions Workshop. The information from this meeting and other sources will provide input to updating the strategic plan for the NNI, which will be undertaken by the Nanoscale Science, Engineering, and Technology (NSET) subcommittee and other federal agency representatives immediately after the overarching workshop. The Nanoscience Research for Energy Needs workshop report also serves to inform further research investments by BES.

Public Law 108-153 and the President’s Council of Advisors on Science and Technology (PCAST) provide oversight for the NNI. Public Law 108-153, the 21st Century Nanotechnology Research and Development Act, was signed into law by the President on December 3, 2003. Among its provisions, the Act formalizes much of the structure that already existed for coordinating the National Nanotechnology Program since 2001. The Act formally establishes the National Nanotechnology Coordination Office, provides for regular external review of the program via the National Academy of Sciences, and indicates that “The President shall establish or designate a National Nanotechnology Advisory Panel” and lists its duties. Prior to passage of the Act, PCAST had already begun to discuss the NNI program and its defining grand challenges in response to the National Research Council’s 2002 review of the NNI. Specifically, it had formed three task forces: Materials/Electronics/Photonics, Energy/Environment, and Biology/Medicine/Societal Issues. On July 23, 2004, the President signed an executive order formally designating PCAST to serve as the National Nanotechnology Advisory Panel required by the Act. PCAST may also come out with some recommendations and directions.

Hemminger was concerned that during the setting up of the nanoscience centers a culture of over-review might be established. With all the workshops, the directors will not have time to do any work and get any science done. Carim replied that not everyone is involved in all these workshops. The grand-challenge workshops are to inform the 5-year plan and will ramp down soon. The meetings among the directors are critical for coordination. More and more of the meetings will be designed specifically for the different types of managers at the centers (e.g., executive committee chairs). Hemminger said that he appreciated the need to get it right, but the need to use people's time efficiently was important, also. Isaacs commented that getting together with the other directors is terrifically important. What is driving all these activities is the science. Perhaps the personnel should get together annually to talk about just the science.

Kohn questioned the use of the term "harvesting of solar energy." One has to distinguish between photovoltaic energy and photothermal energy. Even in photovoltaics, 20% efficiency has been achieved for several years now. The cost of photovoltaic electricity is currently 4 times that of fossil-fuel-produced electricity. The factor of 100 lower cost for photovoltaic electricity that was cited in the presentation must be a typographical error. Williams said that there is no way to get a factor of 100 reduction in cost; it is an aspirational goal.

Cummings said that the recommendation that proposal reviewers look for theoretical-input possibilities was a good one. One also has to judge how access to computer facilities will be assured.

Hemminger introduced a discussion of input for the Theory Subcommittee and the Solar-Energy Workshop.

McCurdy said that the main issue the Subcommittee is struggling with is what the overall model should be: distributed or central, directed vs. blue-sky research, etc. There is a range of opinions among the center directors. From past usages, the phrase "theory, modeling, and simulation" has a certain redundancy between modeling and simulation. More emphasis should be placed on the theory activities. Hemminger suggested that a model based on that of the Kavli Institute for Theoretical Physics at the University of California at Santa Barbara might be good for the nano centers. It would have theorists living in the centers for a significant time but not ensconced as "house theorists."

Cummings noted that the budgeting for the Oak Ridge center allows for three visitors up to 6 months each per year. Kirby stated that one cannot rely on visitors to provide the theory. It is also hard to take off 6 months at a time from a permanent position. Visitor programs are more difficult to maintain because of family needs etc.

Dehmer noted that the theory and computation session of the Subcommittee meeting was the most unsettling. It demonstrated that no one knows how to do it. It was an extension of what the participants already knew. One needs to step back and talk about the range of appropriate models and to talk to people who run theory centers. A full range of possibilities should be looked at before starting the operation of this new type of user facility. The new model might even spill over to all other user facilities.

Stevens stated that this is an experiment in how to operate user facilities. These centers are embedded in national laboratories and should influence the science in those national laboratories (perhaps through joint appointments). The national-laboratory personnel are then collaborators rather than in-house theorists.

Isaacs saw two challenges: critical mass (there are not infinite resources) and top-down vs. bottom-up science. The theorists are not turnkey resources. How to assemble a team of theorists as part of the staff needs to be thought about. Theory as a facility service has to be thought out carefully.

Berrah pointed out that one could think of different ways of attracting theorists. One could invite them to user meetings. The culture needs to be worked on, too. Funding is not given to theorists. A new generation of theorists needs to be nurtured and cultivated.

Kohn agreed with Kirby. Visitors are a good idea. The Kavli Institute for Theoretical Physics in Santa Barbara was a different kind of beast. The NSRCs are also a different kind of beast in their own right. The Institute for Theoretical Physics has five permanent people with tenure in the Physics Department who teach at a one-third level. The other two-thirds of their time is spent at the Institute. They all have graduate students. It costs $3 to 4 million per year. About 40 visitors come in each year. Very few stay 6 months. The median length of stay may be 2 months. DOE needs to be open-minded about how to operate the NSRCs. Kohn had visited three existing theory institutes in setting up the Institute. He learned a *lot* about what *not* to do.

Hemminger moved the discussion to the solar-energy workshop.

Gates stated that biomass conversion needs to be included in solar-energy conversion.

Williams asserted that General Electric must be included; they are staking the future of their company in large part on solar energy. General Electric Laboratories should be represented on BESAC. A true renaissance is occurring at General Electric Laboratories. A detailed financial analysis has been done on solar energy at Hewlett-Packard, which would be of great interest to the workshop participants.

Hemminger asked who the lead contact was for the workshop. Dehmer said that she was.

Kohn pointed out that the Japanese had had the biggest contingent at the recent European conference on solar energy. The Europeans were second, and the Chinese were third. The United States was fourth. The Japanese are not the scientific leaders but are the leaders in infrastructure and use of photovoltaics. They should be involved in the workshop. Germany is leading in organic photovoltaics. Siemens is substantially involved. They have increased conversion efficiency from 2% to 5%.

Hemminger asked for public comment. Douglas Ray pointed out that there is a 6-year example of a facility with an internal theory program, the Environmental Molecular Sciences Laboratory at PNNL sponsored by DOE’s Office of Biological and Environmental Research. He offered the services of his colleagues to advise on the promises and pitfalls of offering such a theory service.

There being no other public comment, Hemminger adjourned meeting at 11:17 a.m.

Respectfully submitted,
Frederick M. O’Hara, Jr.
Recording Secretary
August 17, 2004