Minutes
Basic Energy Sciences Advisory Committee Meeting
February 24–25, 1999, Gaithersburg Hilton Hotel, Gaithersburg, Maryland

BESAC members present:
- Boris Batterman
- Jack Crow (Tuesday only)
- Marye Anne Fox (Vice Chair)
- Thomas Russell
- Barbara Garrison
- Jan Herbst
- Robert Horsch
- Linda Horton
- Marsha Lester (Tuesday only)
- Franklin Orr
- Geraldine Richmond (Chair)
- Stephen Leone
- Zhi-Xun Shen
- Sunil Sinha
- Patricia Thiel (Tuesday only)
- Conrad Williams (Tuesday only)

BESAC members absent:
- Carolyn Meyers
- Ed Wasserman
- David Tirrell

Also present:
- Martha Krebs, Director, Office of Science
- James Decker, Deputy Director, Office of Science
- Patricia Dehmer, Associate Director, OBES
- Iran Thomas, Director, Division of Materials Science, OBES

February 24, 1999

Chair **Geraldine Richmond** opened the meeting at 8:39 a.m. She welcomed the members and asked them to read the report on fourth-generation light sources before the discussion the next day. She had each member introduce him/herself. Richmond introduced **Patricia Dehmer**, Director of the Office of Basic Energy Sciences (OBES).

Dehmer announced that David Moncton had been appointed as director of the Spallation Neutron Source (SNS) and that Bill Appleton had been made Deputy Laboratory Director at Oak Ridge National Laboratory (ORNL). She then reviewed the budget of the OBES. It is the largest component of the Office of Science's budget, with an FY 2000 Congressional budget request of $888.1 million. The actual appropriations in FY 1998 and 1999 were 651.8 and 799.5 million, respectively. The major contributors to the increase in the requested amount were the SNS and BES's portion of the Scientific Simulation Initiative ($7.0 million). She stressed that DOE is a major player in science and a leader in performing research. An analysis of the FY 2000 President's request showed that DOE is in the top five government agencies in support for total research, basic research, applied research, academic research, and R&D facilities.

Dehmer reviewed the mission and fundamental tenets of DOE and cited a definition by which DOE measures all programs: Excellent fundamental research produces new knowledge and ideas that change the way people think, that endure, and that are widely used by others. The research supported by the BES program is recognized as outstanding by peers and is widely used by others. Cited as examples were the work of Paul Boyer on the “energy currency” of the living cell that won the 1997 Nobel Prize in Chemistry, Alexander Pines’s resonance imaging without magnets, and Phillip Paul’s landmark experiment that challenges conventional models of combustion.

BES supports 18 scientific user facilities and 1,400 research projects at 200 institutions. These have come to be thought of as a system of facilities that together serve the national user community, and BESAC has played a major role in our coming to view them this way. Predominant among these facilities are the High Flux Isotope Reactor (HFIR) at ORNL, the High-Flux Beam Reactor (HFBR) at Brookhaven National Laboratory (BNL), the Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory (ANL), the Los Alamos Neutron Science Center (LANSCE) at Los Alamos National Laboratory (LANL), the Stanford Synchrotron Radiation Laboratory (SSRL) at the Stanford Linear Accelerator Center (SLAC), the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory (LBNL), the National Synchrotron Light Source (NSLS) at BNL, and the Advanced Photon Source (APS) at ANL. As an aside, she mentioned that the OBES home page on the World Wide Web has been improved and is now a source of significant information that links the user to these facilities and to relevant Congressional committees.

A comparison of the FY 2000 request with the FY 1999 appropriation showed the following changes in funding (in millions of dollars): SNS, +88.6; construction of Phase II of the Combustion Research Facility, -4.0; the core research program, -17.6, a figure that will be offset by the following two administration initiatives; Climate Change Technology Initiative (CCTI), +11.7; Scientific Simulation Initiative (SSI, initially combustion modeling), +6.8; science education (undergraduate research, faculty training, and K–9 teacher education), +1.9; facilities utilization, +5.7; and Small Business Innovative Research (SBIR)/Small Business Technology Transfer Program (STTR), +0.1. In the core research program budgets, materials sciences, chemical sciences, and energy biosciences are flat, and engineering and geosciences sustained significant decreases. The budgets for the light sources reflect an attempt by DOE to give them cost-of-living increases, and the neutron sources were held flat except for LANSCE and HFIR, which are undergoing upgrades. Russell asked if the trend is away from funding individual researchers and toward funding groups. Dehmer replied that no greater emphasis is being placed on collaborative work but that there is a continuing interest in it. Richmond asked whether people were shifted around when funds are “made up” elsewhere, as with the two new initiatives and the core research program. Dehmer replied that people are not shifted, although continuing programs are in some cases extended or augmented. Not shown in the budget figures is a research initiative in complex and collective phenomena, which is being funded out of OBES funds.

A graph of historic funding levels showed that most of the increase in OBES’s budget between 1988 and 2000 comes from (1) facility operations and (2) capital equipment and construction; funding for base research has exhibited only modest, but fairly constant, increases. Moncton asked if, in the absence of the facilities, the core research would have fared better in funding. Dehmer replied emphatically no, that the core research program has remained healthy largely because of the facilities.

A list of priorities showed the SNS and the research initiative on complex and collective phenomena at the top. The second tier of priorities included maintenance of the depth and breadth of the BES portfolio; scientific simulation and modeling; the Climate Change Technology Initiative; stewardship of neutron-science facilities and communities; extension of the programs and upgrades at the HFIR and LANSCE; expansion of the programs and capabilities at the ALS, APS, NSLS, and SSRL; the upgrades at the NSLS and SSRL; and the R&D agenda for fourth-generation light sources. “On the horizon” were a center for combinatorial materials science and technology and improvements to electron-beam microcharacterization centers. Russell asked if the HFBR was not on the horizon. Dehmer replied that the HFBR has been shut down for more than two years, and since a record of decision is not expected until December of next year; it is currently in hold status.

Dehmer noted in passing that DOE was the leading federal agency in funding for materials science in both 1998 and 1999 and went on to show the different fields that the Department funded and that, nationally, it is a dominant player in both materials sciences and chemical sciences. A bar chart of the total DOE funding for each of the 15 DOE national laboratories (with each bar subdivided to show ER and OBES funding) showed (1) the dominance of the weapons laboratories in total funding and (2) the preponderance of OBES funding at ANL, ORNL, BNL, and LBNL (in decreasing order). This bar chart was indicative of where the Office’s strengths and portfolio are located. Another bar chart that indicated the amounts of funding that had gone to each national laboratory and to off-site researchers divided each bar by program supported and showed that a laboratory does not have to be a dominant player to be an important player.

Herbst asked if the research program in complex and collective phenomena would be a long-term program, and Dehmer said yes, it will be in our base. Leone asked how neutron science could be stimulated, and Dehmer said by helping to support faculty and by paying part of the research funds. Engaging academics in consortia with laboratory people is also desirable. An aggressive program is needed; funding graduate students is not enough. Orr asked if BESAC can help make the case for geosciences and engineering, and Dehmer answered affirmatively. Williams asked about the status of the research program in complex and collective phenomena, and Dehmer responded that the budgets are progressively higher, a workshop will be held at Berkeley soon, and OBES is trying to nurture the initiative. Batterman stated that more academic input to the neutron scattering at BNL might be helpful. Herbst asked Dehmer if her acting directorship of the Office of Computational and Technology Research was distracting from her efforts as Director of OBES. She replied, yes; it takes up extra time, but she has learned a lot about the Office and about computational science and she has gained a lot of allies for OBES.

Richmond then introduced **James Roberto** of Oak Ridge National Laboratory to give a report on the activities of the National Research Council Committee on Condensed-Matter and Materials Physics (CMMP). He started by listing the members of the committee and noted that their charge was to:

Identify future opportunities and priorities in the field;
Articulate the fundamental scientific challenges;
Assess infrastructure, institutional, resource, and educational issues;
Provide evidence of the field’s societal impact; and

Provide a forum for coordinated communications with federal agencies, policymakers, and the public.

These objectives were pursued through a workshop in 1996, committee meetings, an interim report (*The Physics of Materials*), forums at four society meetings, a Web site, a main report (in press), and a forum held in 1999. The interim report was intended for a broad audience to illustrate forefront fundamental research and its impact on our daily lives. The 15,000 copies were distributed to policymakers, academic departments (including every U.S. high school), and members of the American Physical Society. It was used in Congressional and agency hearings and made available on the World Wide Web. The main thesis of the report is that this field's science is close to the cutting edge of technology and affects advances in computers, communications, national security, energy, transportation, entertainment, and medicine.

The final report is a scholarly assessment of the field; one volume of the ongoing decadal review of physics; a summary of impacts, accomplishments, scientific questions, priorities, and policy issues; and a survey of the trends in the field. Its main finding is that this has been a decade of amazing discovery and impact in science and technology - several of the advances have occurred in the last ten years.

In electronic, optical, and magnetic materials, the report focuses on several technological questions, including whether magnetism can be understood on the meso/nano scale, and identifies some major research priorities:

Advanced synthesis and processing techniques including nanostructures and self-assembly;
Physics and chemistry of organic and other complex materials for electronic/optical/magnetic applications; and
Techniques to detect individual electron and nuclear spins at atomic resolution.

Richmond asked what dialog there was between this committee and the chemical and materials community. Roberto responded that the committee viewed the subject as broadly as possible and tried to bring in representatives from these other disciplines. He added that these linkages are extremely important.

The development of new materials and structures holds the question of whether we can complement empiricism with predictability in materials development. Here, the major research priorities are tailoring materials at the molecular level and understanding the physics and chemistry of materials processing on multiple-length scales. Novel quantum phenomena (exhibited by carbon nanotubes, high-temperature superconductors, and other systems) are particularly attractive research priorities as are nonequilibrium physics and soft condensed matter. This last category is witnessing a convergence of physics, chemistry, and biology but not a convergence in language, which is needed so these fields can learn from each other.

Fortunately, new tools for research are emerging, opening up questions about whether we can manipulate single atoms fast enough to make devices, use computation to predict materials phenomena, and image and manipulate spins on the atomic scale. Research priorities for these new tools include:

The Spallation Neutron Source and upgrades at existing neutron sources;
Full instrumentation and exploitation of existing synchrotron sources;
State-of-the-art medium-scale user centers for nanofabrication, electron microscopy, magnetic fields, etc.;
Recapitalization of university laboratories with state-of-the-art fabrication and characterization facilities; and
Exploiting advances in information technology to visualize and simulate materials.

A chart showed that federal R&D expenditures peaked in 1988 and have declined since then. The largest decrease occurred in industry-conducted R&D and was probably caused by the ramp-down of defense spending at the end of the Cold War. A chart of federal investment in condensed matter and materials physics showed a small, but fairly steady, increase since 1985, with DOE funding about twice as much as the next-largest federal agency.

A table of bachelor's degrees awarded in related fields since 1985 showed a decrease in all fields except the biological sciences, which experienced a 44% increase. When broken out, physics enrollments and degrees showed constant declines since 1987 in all categories except PhD degrees, which increased. But new physics PhDs have fallen slightly in the past two years. Women received 13% of physics PhDs in 1996 as opposed to 7% in 1983. First-year graduate students in physics have dropped 27% since 1992; in 1995, 47% of those were foreign nationals, up from 19% in 1970. The average time to complete a doctorate in physics increased from 5.3 years in 1970 to 6.5 years in 1995. The fraction of new physics PhDs in condensed matter remains about the same at about 30%.

At the same time, users at DOE synchrotron facilities increased from almost zero in 1982 to almost 4000 in 1997. Most of these users were in the materials sciences (36%) with the life sciences not far behind (27%).

The Committee recognized that U.S. research universities are a powerful resource for human capital, advancement of knowledge, and the enlightenment of the public. But the research university system faces serious challenges in containing costs while maintaining research infrastructure, attracting underrepresented groups, providing effective outreach to the public, developing curricula responsive to industry needs, and implementing distance learning. The Committee recommended improving the effectiveness of CMMP research and education at universities by:

Reducing the time to complete a physics PhD;
Ensuring broad access to the best research facilities;
Developing curricula that communicate the excitement of CMMP to beginning undergraduates;
Developing graduate curricula that respond to industry needs;
Making physics relevant to U.S. students; and
Improving linkages across disciplines.

At the same time, government laboratories represent a powerful resource for large-scale national missions, multidisciplinary research, and major national facilities. Optimum utilization of this resource requires effective integration with universities and industry, so a broader use of government laboratory infrastructure by universities and industry should be encouraged, and government laboratories should facilitate R&D partnerships with universities and industry. Because the distance between basic research and technological development is small in CMMP, interactions with industry are vital to the development of the field. Such industry interactions with universities and government laboratories include:

Reliance on universities for new CMMP talent to promote innovation;
Industry access to unique skills and facilities;
R&D partnerships; and

Increased reliance on universities and government laboratories as performers of basic research in the physical sciences.

Furthermore, partnerships among industry, universities, and government laboratories provide opportunities for integration of long-term fundamental research, cross-disciplinary teams, synthesis and processing, and strategic intent but require effective procedures for handling intellectual property. These partnerships should be fostered by:

Making resources available through special programs;
Developing effective protocols for intellectual-property issues;
Encouraging internships and sabbaticals in industry; and
Requiring partners to have a stake in the partnership.

The Committee also recommended:

Prompt construction of the SNS and upgrading of existing neutron-scattering facilities;
Increased funding for operations and upgrades at synchrotron facilities;
The broad use of synchrotron and neutron-scattering facilities across scientific disciplines (and correlative budgeting);
Increased investment in the CMMP infrastructure; and
Increased investment in instrumentation and fabrication capabilities.

The strategic scientific themes that the Committee saw emerging during the next decade are:

The quantum mechanics of large, interacting systems;
The structure and properties of materials at reduced dimensionality;
Materials with increasing levels of compositional, structural, and functional complexity;
Nonequilibrium processes and the relationship between molecular and mesoscopic properties;
Soft condensed matter and the physics of large molecules, including biological structures;
Controlling electrons and photons in solids on the atomic scale;
Understanding magnetism and superconductivity;
Properties of materials under extreme conditions;
Materials synthesis, processing, and nanofabrication; and
Moving from empiricism toward predictability in the simulation of materials properties and processes.

Roberto closed with the message that CMMP lies at the heart of revolutionary advances in broad areas of science and technology and has produced enormous societal benefits. Powerful new capabilities in synchrotron and neutron research, atomic-scale visualization, nanofabrication, computing, and many other areas promise exciting new discoveries and are making vast new areas increasingly accessible to fundamental study. Continued leadership in CMMP requires strategic investments in research, facilities, infrastructure, and human capital; the encouragement of discovery and partnerships; and integration of research approaches, institutions, and disciplines.

George Samara of Sandia National Laboratories asked if the CMMP Committee had any idea why the drop-off in physics students occurred, and Roberto answered that they had not gone into such detail. Leone asked if the Committee found any link between job opportunities and degrees granted, and Roberto responded that there are twice as many graduates as jobs in this specific discipline, but *all* graduates are getting good jobs. If you get a PhD in condensed matter and material physics, the probability you will stay in condensed matter is 20% and in physics only 50%; 85 to 90% of the graduates, though, say they would do it again. Dehmer asked if they had made any Congressional briefings. Roberto answered that they had not yet had briefings for the final report, but that the response from the brochure was very positive. The support for science in Congress is strong; the problem is the budget caps. Horsch asked what the Committee recommended about intellectual property. Roberto responded that intellectual property policies are evolving even as we speak. Horsch asked how that will happen, and Roberto stated that, with every negotiation, you start over.

Batterman said that a more insidious factor is that the quality of students in physics has changed; the grades on common or standardized tests are not as good, reflecting the quality of students. Thomas asked if the art was better now than it was 10 years ago, and Roberto responded that very good people can still be hired, but the question is whether they can be offered a good career opportunity. Russell asked for a breakdown between U.S. and foreign nationals, and Roberto said that about half of the hirees are foreign nationals. Sinha said that the same thing is happening worldwide; it is a global problem that people are not going into physics.

A break was declared at 10:45 a.m. Richmond called the meeting back into session at 11:06 and introduced **Iran Thomas** to give an update on neutron-activation-science activities. He commented that OBES has a great responsibility for neutrons but has been doing better by X-rays. The United States has four neutron sources, two of which are spallation sources, half of the world's spallation sources. To improve how neutron science is performed, a workshop on neutron detectors for spallation sources was held in September 1998 at BNL. It concluded that high-intensity sources require high neutron efficiencies, low sensitivity to gamma radiation, and fast (submicrosecond) scintillator response. A new inorganic scintillator material $[(^{6}\mathrm{Li}^{158}\mathrm{Gd}^{10}\mathrm{BO}^{3})^{3}\mathrm{:Ce}]$ meets or exceeds the workshop's requirements. It has a light output six times that of commercial Li-glass and a gamma sensitivity that is 1/1300 that of Li-glass. Such capabilities make a big impact on what can be done with neutrons. Jack Kelley of DOE said that ISIS has been an extraordinary success and asked what its strengths and weaknesses are. Thomas responded that DOE will be sponsoring a national school on neutron and x-ray scattering at ANL in August to pursue this objective.

Thomas noted that the neutron-scattering center at LANL was doubling its power to match that of ISIS and is building new instruments. Ultimately, it will have a 200-μA beam current at 30 Hz to produce 160 kW at 800 MeV and a peak flux that will exceed ISIS's by 1.67. LANSCE is a training ground for the SNS in increasing scientific capabilities through spectrometer development, enhancing user involvement, and enhancing the national capability for constructing neutron-scattering instrumentation.

The SNS is expected to use the model developed by LANSCE, with spectrometer-development teams (including participants from academia and national labs) leading the design, construction, installation, and operation of new spectrometers; LANSCE coordinating the development project; the center having primary responsibility for operation; and a fraction of the beam time being reserved for the spectrometer-development teams. The development teams were invited to submit full proposals, and eight such proposals were received, reflecting a broad representation in institutions and disciplines. The upgrade project will stretch out to 2002. One problem is the limited number of people available to do the required work; as a result, the pool of people that can build instruments for the SNS is being expanded.

No new reactors are being built as neutron sources, so the HFIR is a precious resource for isotope production and for producing high neutron fluxes. The current upgrade is adding a cold source, adding a guide-tube hall, and expanding the number of instruments. The addition of a small thermal guide hall is also being considered. The guide halls will be moved even farther away and will be even larger than originally planned by moving the road that had limited their size. In addition, the new management structure is providing much more reliable reactor operation. As a result, the research community will have a small but very bright cold source and a lot more neutrons. Furthermore, all instruments will meet or exceed the performance of those of the `Institute Laue Langevin` (ILL). The thermal instruments will have neutron fluxes at the sample position that are 1.5 to 10 times higher than currently available at HFIR and up to 3 times higher than available anywhere else in the world. These upgrades will be made during 2000, when the HFIR will be shut down for a replacement of its beryllium reflector.

The Intense Pulsed Neutron Source at ANL (a short-pulse spallation source commissioned in 1981) will continue to operate at its current capabilities.

The High-Flux Beam Reactor at BNL, another of the United States' reactors for neutron scattering, is shut down because of leaks in the reactor pool. The environmental impact statement (EIS) has been delayed at the request of local leaders who have asked for more time for analysis. The earliest a record of decision (ROD) might be entered is December 1999. Garrison asked what was being done to accommodate the users, and Thomas replied that these users (about 200 to 300) have gone to the National Institute for Standards and Technology (NIST) and to foreign sources (such as ILL and ISIS), straining the capacities of those institutions.

The SNS is the future because it is unlikely that the United States will ever build another reactor. The cost has increased to $1.36 billion, and the completion date has been pushed back to the first quarter of 2005 because the FY 1999 appropriation was not as much as had been requested. Reviews of the program indicated that it needed to transition from a conceptual-design and R&D phase to a construction phase, requiring a mix of personnel with different skills and experience than those needed by the leaders of the design effort. Dave Moncton of ANL has accepted the position of project director, reporting to the director of ORNL.

Russell mentioned that public comment at BNL is jeopardizing the whole laboratory, not just the HFBR. Sinha asked if it were true that the BNL management is less than enthusiastic about restart, to which Thomas replied, no, they realize the importance of this facility, but restart is a very daunting task. Crow asked if any assessment had been made of the effect of the shutdown on the graduate-student population. Thomas said that anecdotal evidence suggests that they are discouraged. Russell said that, as he looked at the reports and recommendations, they all say that the reactor should be restarted, and he asked if we are in a situation in which we just have to wait. Thomas responded that there are three components to the Secretary's decision: scientific assessment, community sentiment, and the formal EIS process. Right now, the community input is one of deep concern. Dehmer commented that the collective decision comes from more than just the scientific advice; that is reality. Russell asked if there were anything more that the neutron-scattering community could do. Thomas said that the scientific input is in hand. The problem is that the Long Island community is making it very clear to their representatives that they do not want the reactor restarted. Dehmer concurred.

The chair declared a break for lunch at 12:00 noon. At 1:07 p.m., she called the committee back into session to hear **Daniel Hitchcock** give an update on the Scientific Simulation Initiative (SSI), which is part of the Presidential Information Technology in the Twenty-First Century (IT^2) Initiative, encompassing fundamental research; advanced computing; and ethical, legal, and social impacts. At DOE, the issues addressed within this initiative will be the basic applications (combustion, global systems, and basic science), computer science and enabling technologies, facilities, and management. The basic applications will depend on the development of the computer science and enabling technology, which, in turn, will be based on the computing and communications facilities put in place. The objective is to bring a 4-teraflop machine online by 2000. This project is significantly different from how computer science has been done in the past in terms of what the hardware looks like and how it determines what the code looks like (and vice versa). The applications will have to be coordinated closely. Some of the challenges that must be faced are that terascale computers will be hard to use; current approaches to data management, analysis, and visualization do not scale; ways to enable remote collaboration and use of these resources need to be developed and deployed; many current algorithms scale poorly with problem size; innovative techniques need to be employed, but the applications need stable, engineered tools (some will need to go through three or four generations of hardware without breaking); and the program needs to be balanced among research, development, deployment, and subsequent support.

An indication of the complexities being faced is hierarchy management: Today’s machines have three levels of memory (main memory and two levels of cache); a 10-teraflop machine needs four levels, a 100-teraflop six, and a 1-petaflop seven.

Significant advances in the state of the art are required in many components. Significant research is required just to allow operation of the facilities. The size and disciplinary diversity of the teams are significantly larger than in the past. The time-coupling constant between disciplines is shorter than previously. The software systems are significantly more complex than earlier ones. Managing the complexity is itself a research issue. And all of the pieces of software and enabling technology have to be procured and arrive when the hardware arrives, or the hardware will not work.

A strategic approach will be employed: Software development will be componentized, true partnerships will be forged between the applications and the systems personnel, universities will be involved to develop human capital, and other DOE programs will be leveraged. The computer-science component consists of the development of scalable algorithms, models with improved predictability and reliability, gridding and mesh-refinement techniques, optimization methods, and scalable libraries based on the system components; problem-solving environments, parallel programming tools, debugging and performance-analysis tools, parallel I/O libraries, higher-level language environments, and desktop-based steering and monitoring tools; technology for distributed computing and collaboration (because users will be spread out all over the country); and visualization and data-management systems for managing the data (in datasets of up to tens of terabytes) and interpreting the results.

Horton asked what the distinction was between these common capabilities and the individual needs of the different scientific inquiries. Hitchcock replied that the discipline-related applications must use common tools as much as possible; this boundary will have to be negotiated between the developers and the users.

Because of their high cost, few high-end machines will be produced, but the expertise that will be using them will be located all over the map. This mismatch will be solved by building a computational grid that will link people, computers, data, and instruments, making it irrelevant where the users are. Going to a distributed structure like this presents a number of research challenges:

End-to-end resource management for computing, remote input and output, and visualization;
Global resource management;
Protocols, interfaces, and tools for 100-GB/s networks;
Distributed management of datasets;
Collaborative work by 50-person teams;
Representation and sharing of knowledge; and
Understanding and optimizing performance.

Thiel asked if there would be a centralized office to control how these people work. Hitchcock said there has to be some infrastructure to determine how these people are going to work together, but it has to be lightweight enough to deal with the problem without taking up everyone's time with meetings. Thiel asked if the structure at DOE and the National Science Foundation (NSF) can handle this complex a task. Hitchcock replied that some of these tasks had been explored but are nowhere near this scale. NSF and DARPA (Defense Advanced Research Projects Agency) have been examining how to manage large projects like this one.

Horton asked about the role of the commercial sector. Hitchcock answered that it is hoped that this experience carries over into the commercial environment at the end, but the market for such huge capabilities is so small that the government will have to carry this program to completion on its own. Russell said that he looked upon this project as the same type of vertical management problem as a synchrotron. Hitchcock responded that they are the same except that in this case you cannot see any of the elements that are supposed to come together.

Dehmer asked if he could give an example of any other computer development efforts. He said that there had been some industry-integrated software projects, such as that of Mars Candy. They said that no project could last more than six months. By that time, the business need would have died, and the deadline would force decisions to be made on a basis of pragmatism. Dehmer asked if there had been anything with a significant research component. Hitchcock said that we are moving in a direction that we own; that is what makes it interesting. Shen asked if he could give an idea of what this machine would look like. Hitchcock said that it would look much like the NERSC (National Energy Research Scientific Computing Center), but bigger:

20,000 sq ft of floor space;
1 MW of power;
1 MW of cooling; and
tens of hundreds of petabytes per year that have to be stored somewhere.

William Kirchhoff then spoke on OBES's perspective of SSI, now a part of the administration's \$366 million IT^2 Initiative. Information about this program is available on the Web at www.er.doe.gov/ssi and www.ccic.gov [including reporting on the President's Information Technology Advisory Committee (PITAC)]. The initiative will be coordinated among NSF, DARPA, DOE, NASA, NOAA, and NIH, with NSF serving as the lead agency. Each of these agencies has a different mission, and they determine their research portfolios in different ways, but they share common needs for computational capabilities. Coordination and management plans are currently under development and involve a special principals group for information technology and an interagency working group for information technology R&D. The initiative will support three activities:

1. Long-term information technology research that will lead to fundamental breakthroughs in computing and communications;
2. Terascale computing (10^{12} operations/second with 10^{12} to 10^{15} bytes memory), including the software, networks, supercomputers, and research teams needed to support it; and
3. Research on the economic and social implications of the information revolution and efforts to help train additional information-technology workers at our universities.

The second is the important one for OBES. No program in OBES would not benefit from these massively parallel computers. Because 85% of the nation's energy comes from combustion sources, research on combustion with these computers is expected.

The terascale computational resources and their supporting communications and interfaces will not just be a large NERSC. The complexity of the new architectures that can achieve terascale computing will, for the most part, require a small number of large teams of complementary expertise to make effective use of these resources. At the upper levels of government, it has been decided that:

> All applications will be fully and openly competed and will be peer reviewed;
>
> DOE activities under SSI will involve the DOE laboratories and universities [through parallel solicitations for fairly large efforts by institutions (no individuals), which solicitations will be issued before the appropriation is made]; and
>
> The DOE program will consist of two principal applications (global systems and combustion) plus a basic science-research program that will encompass two to three applications as yet undetermined.

The basic-science activities will be encouraged in but not limited to materials sciences, structural genomics, plasma physics (fusion-energy sciences), high-energy and nuclear physics, and subsurface transport, but other BES applications may emerge, such as catalysis and subclasses of materials sciences. The principal applications (combustion and global systems) will be competed separately with their own notice of intent, and the SSI program will be managed as a project with project-management tools, including change control.

Problems include (1) how to achieve a fully open competition and at the same time a coordinated program with a project-management approach and (2) how to select a small number of successful applications from a diverse scientific background (i.e., how to set priorities).

Thiel asked if combustion modeling will be the biggest or only application. Kirchhoff responded that it was neither; the climate-change effort will be the largest, and there will be others. Dehmer commented that the SSI is different from the CCTI, although the SSI does have a climate-change component, also. Leone said that he could see that they would need faster calculations if they had a fluid flow; but in handling bigger systems, it gets very complex. He wondered how they were going to make the leap to figure out how to solve these highly complex problems. Kirchhoff mentioned a couple of ways, all research intensive. He said that, if we are unable to get rate potential-energy surfaces by any other means than calculations, we are in trouble because of how those calculations scale. But software research can give us better results than bigger and faster calculations. There have to be estimations, but they have to be rigorously tested.

Richmond commented on how this initiative had grown, and asked what can be learned about how to manage it effectively by watching this process. Kirchhoff responded that it is mostly being able to assess the technical problem and determining (1) what you would do with more powerful computers and (2) how you should design a program to address those problems. Lester asked how DOE planned to reach out to the community. Kirchhoff responded that they had been reaching out all along, talking with industry and groups involved with combustion who use big computers; they did not find these people in the national labs. Leone asked how they got the best and brightest workers. Kirchhoff answered, by making a clear announcement of the opportunities, but the issue is going to come to a head when a management structure is needed to deal with the requests from users.

Richmond introduced **Charles Shank**, Director of LBNL, to talk about the upcoming workshop on complex and collective phenomena. The charge for the workshop will come from the Office of Science, and the approach and scope will be determined by OBES. The workshop will be held at LBNL on March 5 and 6, 1999, and an executive summary will be drawn up by the end of March. The purpose of the workshop will be to review a list of preliminary research topics, to identify the scientific challenges (including a vision for the future, a roadmap, and potential endpoints), and to describe possible impacts on society and human welfare. The overall objectives of the workshop are to explore what complex-collective phenomena means, to launch a new science, and to have a major impact on basic-science directions. The chairs of the working groups will be:

Unusual materials: Don Murphy, Lucent Technologies
Control of entropy: Peter Wolynes, University of Illinois
Strongly coupled systems: David Awschalom, University of California at Santa Barbara
Functional design and synthesis: Jean Frechet, University of California at Berkeley
Nonlinearity in space and time: Moungi Bowendi, Massachusetts Institute of Technology

Unusual materials will include materials that are combinations of a large number of elements, are nonstoichiometric, are not at equilibrium, are dimensionally restricted with low symmetry, or are subjected to extreme environments. Control of entropy will consider self-assembly of highly ordered functioning systems, highly ordered living systems, biological processes that produce lower-entropy products (e.g., photosynthesis), and fabrication of mimetic systems. Strongly coupled systems will cover Bose-Einstein condensation, high-temperature superconductivity, strongly correlated electron systems, quantum-phase transitions, and plasma behavior. Functional design and synthesis will include atomic-level fabrication of specific materials, prediction of properties of multicomponent materials, changes in properties produced by changes in atomic composition, and constitutive screening to produce desired properties. Nonlinearity in space and time will discuss nonequilibrium dynamics, plasma dynamics, multiphase flow and reactive transport in geologic media, and seismic and electromagnetic wave propagation in heterogeneous media.

Richmond asked if these topics were developed by the chairs, and Shank replied that these themes will be given to the chairs as a starting point to use or not to use as they see fit. Horton asked what he had decided about the number of people. He said 15 to 20 people, forming a core of leaders that are experts in the selected topics; however, if BESAC is interested in input, anyone who is interested should be allowed to attend. Richmond asked how many will be invited and, of those, how many will attend. Shank said 200 will be invited, and 70 to 100 are expected to attend.

Thomas commented that this is a start of a long campaign about research in the physical sciences. DOE needs to be at the forefront of science and to be able to extrapolate how this is going to affect people's lives and the nation's well-being. We need to step back and contemplate the meaning of what we have seen occur in the past 10 years. As George Washington said in his inaugural address in 1790, "Knowledge is the surest basis of the people's happiness."

Lester asked how the report will be written. Shank said that the five chairs will be the main source of information, and they will be aided by some technical writers. Lester then asked if the workshop would be used to gather information and the core would produce the report. Shank said it was desirable to get the executive summary out by the end of the month so it can be used by Martha Krebs. Lester asked if BESAC could help. Shank replied that all members of BESAC are invited to the workshop and they should forward their input through Iran Thomas. Russell, noting the importance of this report, asked how BESAC could give input on such a short notice. Shank responded that the workshop will not be detailed but would set direction. Sinha commented that, to produce a good report, the chairs should solicit input from others who are not at the workshop. Shank said that they will have that opportunity.

Richmond commented that he should not assume that the chairs will reach out to the broader scientific community and that he needs to tell them to do so; also, the ones who got the original e-mail invitation should also be told that they can send in their thoughts electronically if they cannot attend. She then declared a break at 2:54 p.m.

Richmond called the members back into session at 3:34 p.m. and introduced **Marvin Cassman**, Director of the National Institute of General Medical Sciences (NIGMS), who summarized the study by the Office of Science and Technology Policy (OSTP) of the use of synchrotron radiation for macromolecular crystallography. The study group had four previous reports to build upon. The most recent was published by DOE's Biological and Environmental Research Advisory Committee (BERAC). BERAC had surveyed synchrotron managers about needs and opportunities, and the report synthesized the resulting list.

Concern about availability of synchrotrons to meet the emerging needs began with the observation that demand for access to synchrotrons to carry out X-ray crystallographic studies of biological macromolecules is increasing rapidly. In 1973, about 15% of the structures deposited in the Protein Data Base (PDB) at BNL were determined with synchrotrons; by 1997, that portion had risen to 40%. At the same time, the number of structures deposited rose from about 10 to 1800 per year, an exponential growth.

Although biologists are increasingly heavy users, operational support for synchrotrons comes largely from the physics and materials science sectors of DOE and NSF. Of the six synchrotrons in the United States, four are operated by DOE, one by NSF, and one by the State of Louisiana. Over time, the user group has shifted from predominantly materials science to a substantial portion focused on crystallography in service to the biological community.

The report of the study group made several recommendations for the beamlines serving the biological community:

Increase staffing. A major problem at the synchrotrons is the limited staffing. The BERAC report recommended four staff per beamline, and the OSTP study projected a shortfall of 13 staff members for just the general-user beamlines. About 25 additional staff are being funded this year.

Upgrade the detectors and other equipment. The detectors are slow and outdated, and the beamline optics need improvement. Most of the $5 to 7 million needed to achieve this goal will be in the coming year's budget.

Continue support for R&D. Detector development by the small-business community should be funded, and the National Institutes of Health (NIH) should fund some detector development.

Improve access procedures. No central clearinghouse exists to allocate time for a beamline. Some individual facilities have a central point of access, but not all. Some have burdensome reviews and qualifications, and when access is limited, the question of importance is raised and, in turn, produces more problems. This problem will be exacerbated as demand increases.

Upgrade facility operations. The Birgeneau report has had an effect on operations, as evidenced by NIH's decision to contribute $18.5 million to begin the improvements to the SSRL and NSLS.

Expand existing crystallographic capabilities. A crystallographic beamline should be built at several facilities. The beamlines at CHESS (Cornell High-Energy Synchrotron Source) should be upgraded, superbends should be developed at the ALS, and a new sector should be added to the APS.

These steps will make a big difference to the scientific community. Progress is being made rapidly, but it cannot stop here. Synchrotrons have a broad constituency. Their costs and consequences need to be tracked by the multiple supporting agencies. The demand on synchrotrons is changing rapidly and needs to be tracked.

Herbst asked how long the exponential growth can continue. Cassman said, maybe a decade. It is influenced by two factors: (1) The field used to be the province of a few tinkerers; now the garden-variety biologists are interested in it and have a need for it despite the fact that they are not crystallographers. (2) Structural genomics (high-resolution structure of proteins and functional analysis of genomes) depends on synchrotrons and will increase demand tremendously.

Russell asked what the rate-determining step was in performing this research, and Cassman responded that it was the biosynthesis step of preparing the protein. Russell asked what other techniques are available for this work other than crystallography. Cassman pointed to nuclear magnetic resonance (NMR). Crow asked what the role of X-ray sources would be in the next generation of machines. Cassman pointed out that time-resolved X-ray crystallography is a very specialized technique and that only three places in the world are doing it.

Batterman said that the drug companies benefit tremendously from this work and asked if they were providing their fair share in funding this research. Cassman replied that he was not qualified to comment on it. He did not know how the drug companies should factor into future discussions about building another sychrotron. Certainly, the drug companies are producing targets faster than they can run them.

Crow asked if he saw a growth in the biology or health community where a crystallographer is not the driver of the research employing the crystallography. Cassman responded, yes, they saw a 2:1 ratio of biologists to crystallographers in the user community. Russell asked what the uses were of synchrotron radiation. Cassman said it was used to gain a fundamental understanding of the chemical structure and biological activity. There is a good possibility of describing the structure of the ribosome in the future. Sequence is interesting, but structure is fundamental. Nomics has given us great advances in knowledge, and structural knowledge will give us even greater advances.

Jim Roberto was called upon to describe the HFIR's current activities in light of the August BESAC review reported on at the October BESAC meeting. Roberto reported that, in the past year, HFIR had experienced 1 unplanned outage (vs 5 the previous year), 2 days of lost operating time because of unplanned outages (vs 135 days), two deficiency-in-operation citations (vs 7), a reactor predictability of 98% (vs 54%), and a reactor availability of 63% (vs 46%). Upgrade projects that are under way are the reflector replacement, beam-tube and shutter improvements, installation of the cold source, new beamlines and upgraded instruments, construction of a new guide hall, the installation of a user program, and the establishment of the Joint Institute for Neutron Sciences.

For the reflector replacement and beam tubes, contracts have been awarded for semipermanent and permanent reflectors; final drawings have been completed for the reflector container and pedestal assembly; work is under way on procedures, tooling, reactor mockup, pool clean-out, and development of new techniques for ALARA and personnel safety; the final drawings and design/safety calculations have been completed for the HB-1 and HB-3 beam tubes; safety/design calculations are in progress for the HB-2 and HB-4 (cold source) beam tubes; shutter drawings, safety/design calculations, and design-change documentation are in progress for the HB-1, HB-3, and HB-4; the final report on the pressure-vessel life extension has been completed and issued, demonstrating vessel integrity in the upgraded configuration through 2035; and all the critical-path items are on schedule.

For the cold source, the support building is under construction; the refrigerator has been received; the underground electrical conduits are installed; detailed safety analysis is under way; the moderator vessel specification has been completed and the support structure finalized; and the detail drawings are in progress for the integrated cold source/beam tube assembly. The facility will have a different cold-neutron spectrum than the ILL, ranging from 1.0 to 1.9 times the brightness of the ILL.

For the beam lines and instruments, the conceptual designs have been completed for HB-2 and HB-4 guide systems; the guides' neutron-optics calculations have been completed; the shielding's preliminary designs and calculations have been completed; the thermal guide system has been redesigned to eliminate nonessential guides; the cold guide system has been redesigned to accommodate the cold-guide-hall extension and a second SANS (small-angle neutron-scattering device); the Monte Carlo simulations of instrument performance have been completed for the reconfigured beam lines; the final drawings of HB-1, HB-2, and HB-3 monochromator drums are nearing completion; the instrument upgrades and design are under way; and a proposal for a biology SANS is in preparation.

The expected suite of cold-neutron instrumentation that is expected includes a 35-m SANS with a large-area detector, a cold triple-axis spectrometer, a biology SANS instrument, an ultrahigh-resolution SANS, a reflectometer, and a truncated 12-m SANS. The expected suite of thermal-neutron instrumentation includes triple-axis spectrometers for the HB-1, 1A, 2, and 3; a residual-stress spectrometer; a wand spectrometer; a powder diffractometer; a 4-circle diffractometer, and a sample-alignment station. All instruments will meet or exceed ILL performance.

The construction of the Neutron Sciences Support Facility is under way with a planned completion date of November 1999. The access road was rerouted to accommodate the cold-guide-hall extension, and the preliminary proposal and cost estimate for the extension have been completed.

The inaugural meeting of the SNS/HFIR User Group was held in Knoxville in November 1998, and program planning is continuing with user involvement and facility benchmarking. The conceptual design for the Joint Institute for Neutron Sciences (JINS) was completed, and a new site was identified. The JINS is an $8 million facility funded by the State of Tennessee, a joint HFIR/SNS user support facility. The guidelines for JINS operation have been developed with The University of Tennessee, and a search is under way for the JINS director.

A review of the current status of the HFIR upgrades showed the cold guide hall and the cold-source support facility under construction; the pressure-vessel life-assurance final report issued; the beryllium reflectors in fabrication; the reflector pedestal and cage in procurement; the HB-1/HB-3 beam tubes and shutters and beam tube in procurement; the cold-source refrigerator on site; and the neutron guides, instruments, beamlines, monochromator drums, and proposed cold guide hall extension in design.

In October 1998, BESAC recommended that a plan be developed to address the long-term reliability of HFIR, a vision be developed of the expected outcome of the upgrades and a management plan be implemented to reach that goal, a high-quality user program be developed for the upgraded HFIR and the SNS, a plan be developed for staffing, and close coordination be maintained with the irradiation and isotope communities to ensure that their needs are met to the maximum possible extent. Each of these issues has been or is being addressed:

> A comprehensive long-term-reliability plan has been developed, capital-investment priorities have been established through 2005, resource requirements have been established for operating budgets, and the plan has been presented to BES.
>
> Clear priorities that meet or exceed performance expectations have been established for the HFIR and the upgrade projects with the aid of community input, performance goals have

been refined and validated, a comprehensive project-planning model has been implemented, and reactor-interface issues have been identified and addressed.

A two user groups (one specifically for transuranic-isotope users) have been chartered, and new procedures are being developed to handle increased user demand.

User-community involvement has been enlisted through user groups; the JINS; external advisory committees for key projects; instrument-development teams; and broad communication through newsletters, workshops, and presentations.

The HFIR staffing profile has been benchmarked against other neutron-scattering user facilities, the staffing plan was updated to incorporate BESAC's recommendations, scientific/technical staff per instrument will be increased from 1.9 to 2.4 in the next three years, the upgrades advisory committee was broadened to include biological interests, and The University of Tennessee will provide 10 new faculty positions during the next 5 years.

An assessment of whether these upgrades and changes are having any adverse impacts on the isotope and irradiation communities showed that the neutron-scattering upgrades do not affect reactor access or performance for isotope and materials irradiation experiments; the reactor schedule and core/reflector experiment loading is being coordinated by a committee representing operations, neutron scattering, isotope production, and materials irradiation; and the proposed pool-side hot-cell facility will not interfere with the neutron-scattering upgrades.

He summed up his presentation, saying:

Significant improvement was made in HFIR availability and predictability in 1998.
Upgrade construction projects and major procurements are on schedule.
A detailed cost/schedule/resource-loading model is in place.
A SNS/HFIR user group has been established.
Specifications and operating guidelines have been developed for the JINS.

Thom Mason then gave a presentation on the users and science of the SNS. The users were dealt with first, stressing that SNS will be a *user* facility. There is, or will be, user input into the instrument suite; an Instrument Oversight Committee (IOC) and workshops; technical, scientific, and logistical support for experimenters; and a peer-reviewed proposal system. HFIR will be used as a proving ground for these approaches before the SNS attracts 1000 to 2000 users per year from academia, government, and industry. HFIR and the SNS will share a unified proposal-submission process.

The user workshop held in November 1998 provided an update on SNS and HFIR, set priorities for the initial instrument suite at SNS, made the science case for a second target/instrument suite, and established a combined SNS and HFIR users group. More than 200 participants from government labs, universities, and industry registered for the workshop. They drafted a charter for a joint SNS–HFIR users group, and on the basis of the priorities identified by the users, the IOC recommended that work begin on conceptual designs for:

A third-generation powder diffractometer with a resolution d/d of ~1 x 10^{-3} at 90 ;
A high-speed, single-crystal diffractometer with energy discrimination;
Reflectometers;
A crystal-analyzer spectrometer with an energy resolution of <10 µeV; and
A chopper spectrometer with an energy resolution of ~1% of the initial energy.

Instrument selection will begin in July 1999 with a presentation of candidates based on this list. The IOC discussed: (1) the importance of the long-wavelength target-station initiative; and (2) staffing of the instrument-scientist positions (six people have been hired, and three more will be hired by year's end). It also indicated that, in examining trade-offs between performance and number of instruments, any instrument built at SNS should meet or exceed the capabilities of comparable instruments at other facilities with constant flux.

To get some idea about what kind of scientific program might be conducted with the SNS, he reviewed some of the things being done now:

> In engineering materials, strain scanning at depth in welds with a pulsed source gives full-diffraction profiles vs the x-y-z coordinates, allowing residual stresses to be recognized. With the SNS, gains in source performance and instrumentation will translate into an ability to do diffraction imaging with sub-mm^3 resolution to visualize strain, composition, texture, and plastic-deformation history.
>
> At the NIST, a cold-source neutron beam (NG1) is polarized, and its reflection produced by a glancing incidence upon a sample is analyzed to provide information about the incident surface. The molecular beam epitaxy chamber in that same beam provides a number of capabilities (protective environment, epitaxial thin-film growth, gas loading, sputter etching, reflection high-energy electron diffraction analysis, and mass spectrometry); allows the use of a number of scattering techniques (specular reflectometry, off-specular scattering, grazing-angle diffraction, high-angle diffraction, and SANS); and allows the study of several phenomena (adsorption/desorption, diffusion, segregation, morphology, crystallography, magnetism, and superconductivity). In addition to providing a unique probe for magnetic surfaces and multiple layers, polarized neutrons permit direct inversion to obtain the scattering-length density profile with no phase problem. One would also like to be able to do off-specular reflection for in-plane structure.
>
> High-resolution spectroscopy with cold neutrons is performed at ISIS with a backscattering technique.
>
> At LANSCE and NHMFL (National High Magnetic Field Laboratory), extreme sample environments are probed in a 30-T, 2-Hz device with a 5-mm slit and a 2-mm bore by phasing the magnetic field to the neutron pulse. This technique is prototypical of the stroboscopic use of a spallation source. In such extreme-sample environments, neutrons already push the boundaries at nK, pK, and kK; 30-T; 25-Gpa; and corrosive, explosive, and aqueous environments. Time-of-flight techniques are well suited to extreme sample environments.

Richmond opened the floor to public comment. Richard Goldstein of the University of Minnesota expressed great concern about the very significant decrease in funding for engineering and geosciences in the core program and urged BESAC to support these programs.

The chair adjourned the day's session at 5:21 p.m.

February 25, 1999

Chair **Geraldine Richmond** called the meeting to order at 8:52 a.m. and introduced **Martha Krebs**, Director of DOE's Office of Science (SC), who reviewed the Office's goals, themes, budget and program priorities, and challenges. She described a series of workshops in which the participants (1) discussed how to move the Office toward the broader ambitions of the Department and (2) began development of a strategic plan on how to get there. What evolved was the identification of five themes:

Fueling the future with affordable and clean energy;
Protecting our living planet against adverse energy impacts;
Exploring matter and energy;
Developing extraordinary tools for extraordinary science; and
Enabling science through supportive institutions and management.

These themes were stated in terms of objectives from which could be derived some investment strategies for achieving these objectives.

Under the leadership of Undersecretary Ernie Moniz, DOE tried to capture the detailed R&D activities of the entire Department ($7.4 billion) to connect them with the budgetary investments. He wanted to provide a clear story of why each of our missions depends on R&D investments, a connection that is not always clear because disparate disciplinary influences, organizational interests, and political interests make it difficult to keep straight what is going on. The challenge was to go into the details of the budget and to roll those details up into these five themes. The program managers were asked to lump their 93 program areas by their support for these themes. The higher-level program managers were then asked to rank these activities by their support of the major themes or challenges. Thus, we were able to identify *and convey* the types of research investments being made in response to the challenges. Unlike the rest of the Department, SC was allowed to double count because of the cross-disciplinary nature of its work. This document will continue to be formulated because it conveys how much of the work that the Department does (the work that the scientific community cares about) relates to the missions of DOE. Now the program can be justified to a degree that was never attainable before.

Shifting the focus to the budget, Krebs displayed the Office's funding history for fiscal years 1998, 1999, and 2000, which showed an increase of 8% in FY99 and an increase of 5% in the FY00 request. Within that, the OBES budget went from $651.8 million in FY98 to $799.5 million in FY99 to $888.1 million in the FY00 request. The bottom line is actually pretty good, a remarkable turnaround in fortune in terms of where SC started the year. Of the $184 million increase in the current request, $84 million is for the SNS, $70 million for the SSI, $10 million for science education, $11 million for biological and environmental research, $7 million for neutron physics, and $1 million for program direction. The funding for the new CCTI is embedded in these figures.

From the budgetary viewpoint, what the Department is going to focus on in the future are the SSI, SNS, science facilities utilization, the Large Hadron Collider (which is in very good shape), and the next-generation Internet (for which $15 million was added at the last minute of the FY99 budget discussions). From the science viewpoint, it is going to focus on the SSI, CCTI, human and microbial genomes, neutrinos and dark matter, and science education (which was budgeted for $4.5 million in FY99 and has a FY00 request of $14.5 million embedded in the program-direction funds).

The SSI is part of the President's information technology initiative; DOE has $70 million of the $366 million interagency program, a partnership with DOD, NSF, NASA, NIH, and NOAA. DOE will carry out its part in this initiative through a partnership with the Accelerated Strategic Computing Initiative (ASCI). This is really a twofold activity. Teraflop-scale facilities are needed and being pursued for nuclear-weapon stewardship. But if you could bring this computing power to the broader scientific community, it would open up not only the science but also a great social contribution. The Department, especially SC, has a number of challenges in the scientific arena that such a capability could help address:

> Climate change is certainly a broad concern.
>
> Combustion is not as widely recognized but as important. EPA is projecting zero emissions from transport vehicles by 2050, but we do not know how to produce such devices.
>
> Clearly, there will be an impact on the basic science areas of structural genomics, fusion energy, materials sciences, high-energy and nuclear physics, data management, and subsurface flows.

The DOE project is considering the foreseeable future, and looking at the terascale with hundreds of users at five centers of excellence. The President's initiative is considering the barely imaginable future and looking at the petascale with billions of devices on the system.

The SNS is the most important project ever for materials science, for the laboratories, and for OBES. It needs to be brought in on time and on budget. Although the timing was awkward, the recent review by the General Accounting Office (GAO) pointed out problems that needed to be solved. Those changes have been made, and the scope and responsiveness of those changes are a testament to the quality and credibility of the reviewers. We were fortunate in being able to impress Dave Moncton into service as the project's director. The Department is now in a strong position to go back to the Hill, having addressed the GAO's concerns.

She had been briefed by Jack Crow on the HFIR review, and said it is now clear that there is an opportunity here to pull together a real vision for the neutron-science community. She attributed this situation to BESAC's work.

Herbst, noting that the SSI is very ambitious, asked if DOE can get the interagency cooperation to pull it off. Krebs replied that this is new money in both the NSF and DOE, and the major differences between the agencies are culture and how each invests in the community. There is $34 million for infrastructure, which is very comparable to the investments the Department wants to make. A joint solicitation and review will be conducted that focuses on collaboration between national laboratories and universities. In the enabling technology area, joint solicitations and reviews will probably be conducted, also.

Sinha asked if the bottom-up budget numbers that she gave were subject to cuts by Congress. She said that the response on the SNS is remarkably steady; Congress seems to understand the importance of the facility. Shen asked what concerns she had about the budget. She said that high-energy facilities (demands for a heavy-ion collider and the synchrotrons) have increases that we have to work hard at to maintain. The user facilities are the topic of confusion and contention, so they are always a source of worry. They worry about the balance between the core research and the facilities. She noted that you can never feel good about the proposed budget. Representing the diversity of interests represented by the user facilities is very difficult.

Richmond said that BESAC would like to help her argue for the base budget. Krebs replied that this is a perennial script. On another subject, she pointed out that the $184 million increase in the budget is more than a cost of living increase; it is largely the SNS and the SSI. The "cost of living" increase is distributed across the programs. The question is how to mobilize the community from the bottom up.

Richmond introduced BESAC member **Stephen Leone** to report on the activities of the BESAC Panel on Novel Coherent Light Sources. He listed the names and affiliations of the members of the panel and the laboratory liaisons who had been invited to the meeting of the panel, which met in a workshop format January 18-22, 1999, in Gaithersburg, Maryland. The panel had been asked to assess what new DOE science may become accessible through new light sources based on advanced concepts, including synchrotron-based methods, free-electron lasers, table-top laser systems, and undiscovered methods. The panel's discussions were to be tempered by the expectation of limited government funding, assuming that only a few, excellent, large-scale proposals will be funded in the future. Before the workshop, the panel examined extensive documentation and previous reports. The workshop involved major presentations by representatives from seven DOE laboratories and by six invited experts on table-top laser light sources.

The panel found the most exciting potential advance for innovative science is most likely to be in the hard X-ray region, in the range above 8 keV. New experiments might include:
time dynamics coupled with structural information;
possible holographic imaging; and
multiple-photon processes at very short wavelengths.

The panel was not unanimous in whether all of these techniques would work, but it was unanimous in its recommendation that a more effective case for the science needed to be made through early and close interactions between X-ray source developers and prospective users.

The panel found that the development of fourth-generation light sources will likely be based on a self-amplified spontaneous-emission principle in a linac-driven free-electron laser or on a seeded, amplified stimulated-emission free-electron laser. The improvements that have been made in the necessary electron-beam parameters are sufficient to warrant cautious optimism that such a device can be built with additional research and development of numerous crucial aspects, such as:
electron-beam emittance and transport;
interaction of the electron beam with radiation;
beam compression; and
laser gain, saturation, and wavelength and their scalings.

The panel expressed an expectation that a strong symbiotic relationship will exist between future accelerator-based sources and high-powered, ultrafast lasers. Lasers are necessary for photocathode drivers, seeding, and possibly electron-beam slicing, as well as for driving the time

dynamics of the science performed (i.e., a pulsed laser will most probably be used to initiate processes that are probed by coherent X-rays). It noted that pulsed table-top lasers have made remarkable progress, achieving shorter wavelengths, higher powers, and shorter pulse durations; and that they are on the verge of producing readily available attosecond sources of soft X-rays. These developments virtually ensure that any light-source facility of the future will include a marriage of accelerator principles and laser art.
The main recommendations of the panel were:

- Establish an early and strong coupling between scientific users and source developers.
- Take tightly focused and fiscally responsible steps to determine the feasibility and design of a 1.5-Å coherent light source.
- Design and develop key scientific experiments that can be achieved with such a new source.
- Provide independent and vigorous support for the development of laboratory laser sources in unique time and wavelength ranges. Remarkable developments are occurring in this area, and these devices will become integral components of the equipment.
- Use third-generation sources and table-top lasers as proving grounds for innovative science and experiments planned for future light sources.
- Support the development of new forms of X-ray detectors and optics.

Leone then displayed a copy of the full recommendations from the panel's draft report and opened the discussion to questions. Russell asked if investing in these sources wasn't necessary due to the overwhelming benefits of the equipment. Leone responded affirmatively, but cautioned that the powers could be too high and might damage the samples. Russell asked if there were any estimates of the cost of the equipment. Leone said the development of the free-electron laser principles might cost up to $8 million per year just for exploratory work, pre-electron laser might cost up to $8 million per year for just exploratory work, the LCLS [Linac Coherent Light Source] might cost $100 million to demonstrate at SLAC, and an actual user facility (a superconducting device with 20 conductors focused at <1.5 Å) might cost several billion dollars and be built in 10 to 15 years. Russell asked how many researchers might use such a facility, and Leone responded that a real facility might support 20 users at a time.

Batterman commented that, at the meeting, he gained a great respect for lasers, but felt that there is still a need to define what types of experiments would be done on such a machine. In earlier projects, there were some real surprises in what could be done. For example, synchrotron radiation ended up to be a great benefit to protein crystallography. When a venture like this is launched, it is likely that there will be serendipitous technical surprises and associated explosions in demand as people realize what can be done. He recommended that the Panel's demands for specific experiments be reduced and that a philosophy of "if you build it, they will come" be adopted. He said that this equipment offered extraordinary opportunities and should not be turned down.

Leone recapitulated the cautions:

1. The damage done by the pulse is a potential problem; 40% of the sample would likely be lost in the first pulse.
2. We must all expect to have peer review.
3. The high cost of the facility means that the scientific output requires considerable justification.

To these, Richmond added a fourth: Clearly, there is not enough communication between the laser people and the facility people; the opportunities for discovery that the laser people bring may not be recognized if the dialogue is not fostered.

Shen commented that the major discoveries to come out of such new capabilities are not the ones that are expected. Herbst told Leone that he had done a magnificent job; he felt that it was wise to couple some of the people with science ideas with the facilities people. You cannot construct a machine without listing some of the things you are going to do with it, even though some are dependent on breakthroughs. Sinha observed that one of the solid contributions of the workshop was the realization of the potentials of other disciplines. With the third-generation machine, the initial "scientific justifications" did not include some of the most important contributions that have come out of them: coherence, nuclear Mössbauer scattering, and microfocused beams. Fox said that if you did not have unexpected developments, you would not have anything worthwhile. She expressed the opinion that you must have science people involved in the equipment design and said that the Panel had done a good job at that.

Horton reinforced the suggestion that OBES should fund the investigatory phase, but that a stronger scientific case would have to be made for the $100 million expenditure. Russell said that the community should start thinking seriously about justifying the pursuit of this path of development. Sinha said that he expected that to occur during the next couple of years. Richmond commented that this report is a good starting point for that discussion. Batterman cited a statement on p. 20 of the report ["(c) the compelling ... within two years"] and said that found this statement too strong. Leone replied that it means that in two years there should be a reality check and that most of the laboratories agreed. At that point, it might be found that source development may require three more years.

Richmond asked for a vote to accept the report as written and to forward it to OBES. The vote was unanimous to do so. A break was declared at 10:45 a.m.

The meeting was called back to order at 11:17 a.m., and **John Stringer** of the Electric Power Research Institute was introduced to speak on centers for the development and employment of electron-beam microcharacterization. He is the chairman of a panel that is being assembled to assess the promise of such centers, and the purpose of his presentation was to introduce the topic to BESAC, and to get its guidance on how to progress. He noted that science has three related tools for studying matter: photons, neutrons, and electrons. Each has a role to play, and each can do some things better than either of the others. For example, neutrons were used for the first crystallography of high-temperature superconductors, but electrons were used to investigate the pinning centers and the role of impurities.

Electron-beam imaging and characterization began with Gabor's chance observation of an imaging effect in a cathode-ray tube and subsequently included:
  the development of a practical electron microscope by Ruska;
  the demonstration of electron diffraction with these machines in 1927;
  the development of the standard bright-field method by Boersch in 1936; and
  the production of scanning electron microscope images in 1942.
The scientific advances made possible by this technology include:
  X-ray crystallography;

physical metallurgy;
microstructural chemical analysis; and
the detection and measuring of dislocations and their interactions with grain boundaries, small particles, and other dislocations.

Two advances that significantly furthered the technology were the development of electropolishing for preparing electron-transparent specimens from bulk samples and the development of advanced specimen stages.

A center for electron-beam microcharacterization might house cutting-edge or unique instruments, develop new techniques and procedures, provide expert staff for the application of the equipment and techniques, train users planning to purchase new equipment, and foster synergisms among specialists with different interests and backgrounds.

To determine whether such a center would be justified, the panel has been asked to assess:
the scientific and technological impact of extant microcharacterization centers during the past decade and their expectations during the coming decade;
the current user demand and how is it expected to change;
the special needs each of these centers serves;
how the centers complement one another;
the vision of each center and whether the visions are appropriate and complementary; and
the opportunities for improving techniques.

To make such an assessment, the panel should meet with the managers of the various centers and should talk with users to determine the degree to which the user communities are being served. The panel should be made up of two types of members, those familiar with the science of electron-beam microcharacterization (who can judge the future opportunities) and those familiar with the techniques (who can assess the current status and future needs in the centers). Representatives of the various centers will participate in some discussions, but will not be voting members and will be asked to withdraw from discussions related to the specifics of the performance of the centers.

Stringer noted that the microscopes supported by NIH would be excluded because their work is very different from that of materials science. The panel would look at polymer research but not at biological substances. Each technique has its own contribution, so the panel would have to cover each of them. He asked for input on the size of the panel, the methods to be employed, and the scope of the effort.

Richmond suggested that BESAC draw up a list of potential members as a starting point for naming the panelists. Stringer noted that including some Europeans and non-U.S. North Americans might be desirable. Asked of the timetable, he said the Materials Research Society meeting in April would be used as a dry run, the list of accomplishments would be drawn up by the labs by mid-May, the visits would be conducted in early June, additional information would be pulled together by the end of June, and the report would be presented to BESAC at the August meeting. Russell noted that several electron microscopy centers are funded by NSF and that NSF should be able to suggest the names of some potential panel members.

Richmond turned to old business, noted that Tom Russell and several others are rotating off this group, and thanked them for their service. Under new business, she noted that the next meeting would be August 10-11, 1999, and the following meeting would be October 25-26 or October 26-27. She then opened the meeting for public comment.

Denis McWhan of BNL added his appreciation for the work of the fourth-generation light-source panel, although he was disappointed that they did not want to support a free-electron laser in the ultraviolet. He noted that BNL has a facility that will be coming online, and a users group will soon be determining what experiments should be conducted. After that, the panel may want to reconsider its recommendations. He also noted that DOE supports several electron-microscopy facilities and said that the microcharacterization committee should survey those facilities to assay user demand.

The meeting was adjourned at 12:17 p.m.

F. M. O’Hara, Jr., 5/5/99

revision by L. L. Horton, 7/1/99