Minutes for the
Basic Energy Sciences Advisory Committee Meeting
October 26-27, 1998, Gaithersburg Hilton Hotel, Gaithersburg, Maryland

BESAC members present:

Boris Batterman
Jack Crow
Barbara Garrison
Linda Horton
Stephen Leone
Marsha Lester
Carolyn Meyers
Geraldine Richmond (Chair)
Thomas Russell
Zhi-Xun Shen (Tuesday only)
Sunil Sinha
Richard Smalley
David Tirrell
Conrad Williams

BESAC members absent:

Marye Anne Fox (Vice Chair)
Jan Herbst
Robert Horsch
Franklin Orr
Patricia Thiel
Edel Wasserman

Also present:

Patricia Dehmer, Associate Director, ER, OBES
Iran Thomas, Deputy Associate Director, ER, OBES
and Director, Division of Materials Science, OBES

October 26, 1998

Chair **Geraldine Richmond** opened the meeting at 8:20 a.m. She explained that Martha Krebs was to have addressed the meeting, but had been called away for another commitment. She announced that the agenda would be rearranged to provide a reading period for each member to review the BESAC Panel report on the High Flux Isotope Reactor (HFIR) at Oak Ridge National Laboratory (ORNL), which would be presented later in the meeting by Panel Chair Jack Crow. She had each committee member introduce himself or herself. She then declared a recess for the reading period.

At 9:30 a.m., Richmond called the session back to order, commended Crow and John Stringer (HFIR Panel Vice-Chair) for their work on the HFIR review, and introduced **James B. Roberto** to provide an overview of the HFIR, the installation of the cold source, the replacement of its beryllium reflector, and its neutron scattering projects. He explained that the HFIR initiated operation in 1966. It produces the world's highest steady-state thermal-neutron flux at 2.3 x 10^{15}n/s-cm^2 in the central flux trap and 1.2 x 10^{15}n/s-cm^2 at the end of the beam tubes (at 85 MW). It has a highly flexible design to serve multiple missions. It possesses outstanding capabilities for neutron scattering, isotope production, materials irradiation, and neutron-activation analysis with four large beam ports and 12 neutron scattering beam lines, 70 target positions, and unique capabilities for transplutonium-isotope processing and research. It is expected to provide full-power operation through 2035. He described the facility and its

buildings and their functions; the design, operation, and configuration of the reactor; and the replacements and upgrades that need to be performed.

Roberto pointed out that HFIR users conduct neutron scattering for fundamental research and materials development; production and processing of transplutonium isotopes for medical, industrial, and military applications; irradiation, testing, and modification of materials for future energy options and commercial applications; and neutron-activation analysis for environmental, industrial, and forensic applications. He presented the number of users for each of these activities by type of user (university, industrial, etc.); the total number of researchers and industrial companies that typically use the facility this past year is about 400. That number is expected to exceed 750 after the replacement of the beryllium reflector and operation of the cold source.

He detailed the transplutonium isotope processing and research being done at the HFIR. The HFIR/Radiochemical Engineering Development Center (REDC) complex is unique in the western world for the production and chemical processing of transplutonium isotopes. It provides isotopes for basic research on the physics and chemistry of heavy elements and actinides. Elements 104, 105, and 106 were discovered with HFIR/REDC materials. More than 100 ^{230}Cf sources are currently on loan to 63 institutions that use them for heavy-element research, medical studies, classroom instruction, and industrial and military applications. Major uses of californium include reactor-startup sources, nuclear medicine, fuel-rod scanning, neutron radiography, and neutron-activation analysis. A major achievement is that californium sources in clinical trials have increased five-year survival rates for certain cancers by 60%, with a concomitant saving of over 360 lives. In the course of these efforts, REDC has forged important partnerships within DOE and with other federal agencies, providing diagnostic materials, transuranic-waste-treatment technologies, and ^{238}Pu power systems.

Roberto provided additional detail about HFIR's contributions to medical isotope research. More than 10 million diagnostic and therapeutic uses of medical radioisotopes occur annually in the United States. Substantial growth (particularly in therapeutic use) is expected during the next decade. Reactor-produced isotopes are "neutron rich," decaying by beta emission, which is important in therapies because these need large amounts of energy to be deposited at the target site. The high thermal flux of the HFIR is important for providing materials with high specific activity. HFIR isotopes are currently in 24 medical trials worldwide; examples are ^{188}Re for inhibition of arterial restenosis and bone pain palliation, ^{117m}Sn for bone-pain palliation, and ^{186}Re for bone-pain palliation. An important issue for medical radioisotope research and use is the predictability of supply (which translates into reactor availability).

Roberto stated that HFIR has faced two recent challenges: an increasing number of minor occurrences resulting in loss of reactor operating time and an increasing concern from facility customers (DOE and users) about decreased reliability and predictability of HFIR operations. He showed a graph of operating availability. The maximum availability is 70%; for the past two years, HFIR's availability has hovered around 45%.

In response to these challenges, ORNL conducted a Laboratory-initiated self-assessment of factors contributing to the reduced availability of HFIR and failure to meet customer

expectations; addressed self-assessment recommendations at the Laboratory, division management, and operational levels; found that reactor availability was most impacted by aging equipment and infrastructure; conducted a national search for a new division director; and operated HFIR successfully for the past seven months. The assessment found that refurbishment of the secondary cooling system (particularly the cooling tower) is urgently needed. Other high-priority needs are:

- Refurbishment of the normal emergency power system
- Upgrading of the instrumentation and controls
- Refurbishment of the main coolant pumps
- Replacement of control-plate-drive systems
- New heating/ventilation and air conditioning (HVAC) system, primary heat exchangers, air-treatment system, and fire-protection alarm system

Reactor safety and technical capabilities are not impacted by these problems, but reactor reliability is.

Reasons to make such investments in HFIR include:

- HFIR has the world's highest thermal-neutron flux.
- Using modern cold-source and neutron-guide technology, HFIR can provide the world's most intense steady-state beams for neutron scattering research.
- Modest investments in HFIR can ensure availability through 2035 with no changes to the pressure vessel.
- HFIR provides unique capabilities in many areas of isotope production, neutron scattering, materials irradiation, and neutron-activation analysis.

Improvements currently under way or proposed include replacement of the beryllium reflector, replacing beam tubes, installing the cold-neutron facility, installing the thermal-neutron facility, and upgrading the instrumentation. A pressure-vessel life-assurance test program will demonstrate vessel integrity under worst-case conditions until approximately 2035; moreover, the design of the upgraded HFIR conservatively satisfies Nuclear Regulatory Commission criteria for vessel failure during power-reactor operations.

Roberto then reviewed the relevant history of proposed neutron scattering facilities: In 1993, the Kohn Panel pointed out the critical need for a complementary pair of sources: a new reactor [later called the Advanced Neutron Source (ANS)] and a 1-MW pulsed spallation source, stating that any plan not including a new high-flux reactor was unsatisfactory. In 1995, the ANS was terminated because of budget constraints, and the construction of a next-generation pulsed spallation source was recommended. To meet reactor facility needs, the High-Flux Beam Reactor (HFBR) and HFIR proposed complementary upgrade proposals. In 1996, the Birgeneau Panel recommended that DOE proceed immediately with the proposed HFBR and HFIR upgrades, stressing the complementary nature and uses of reactors and pulsed sources. HFIR's cold source was subsequently funded in FY 1996, and the replacement of its beryllium reflector (including enhanced neutron scattering capabilities) was funded in FY 1998.

The HFIR cold source conceptual design has been completed, and a report on it has been issued. A preliminary safety analysis has been completed. Loop testing has been completed, and the final design is under way. The delivery of a $1.9 million refrigeration system is expected in December 1998. The design of the support buildings is completed, and site preparation is under way. He compared the cold-neutron brightness of the HFIR and the ILL (Institute Laue Langevin) and showed that the capabilities are quite close. He pointed out that the centerpiece of the facility is a 35-m small-angle neutron scattering instrument with a large-area detector; unfortunately, it is located only 120 ft from the core because of the presence of a road past the building, which degrades its signal-to-noise (S/N) ratio. When the road is moved and beam line can be reconfigured, the S/N ratio will be much improved.

Turning to the thermal-neutron guides, Roberto pointed out that HFIR had made substantial improvements in beamline design which will increase the neutron intensity up to a factor of three. Upon completion of the upgrades, this facility will meet or exceed ILL's performance, although HFIR will have 14 instruments compared to ILL's 40.

The replacement of HFIR's beryllium reflector is being coordinated by a steering committee that reports at the ORNL associate-laboratory-director level. There are two project leaders and a scientific director. The committee oversees more than 2000 individually scheduled activities that involve placing dozens of specialty procurements and fabrication/construction contracts, many of which require many one-of-a-kind designs. Progress is tracked with a five-level work breakdown structure.

Roberto cited the FY-1998 accomplishments:

- The cold-source reference-design report was issued.
- A request for proposals (RFP) was issued, and a contract was awarded for the Neutron Sciences Support Building (NSSB).
- An RFP was issued, and a contract was awarded for the cold and thermal guides.
- An RFP was issued, a contract was awarded, and construction was completed for the modular HFIR-user-support facility.
- The safety analysis and approvals were completed for the new reflector, and an RFP was issued.
- The vessel-life-extension analysis was completed, and a letter report was issued.
- An RFP was issued for the cold-source building.
- The beam-tube designs were 75% completed.
- The beam-line and instrumentation layouts and performance estimates were completed.
- The requirements document was completed for the Joint Institute for Neutron Sciences (JINS).

Roberto then outlined the FY-1999 plans:

- The beam-tube designs and safety reviews will be completed, and the RFPs will be issued.
- The cage modifications and safety review will be completed, and an RFP will be issued.
- The monochromator-drum designs will be completed, and the RFPs will be issued.
- The final report on vessel evaluation will be issued.
- NSSB construction will be completed.
- The cold-source support building will be completed, and the refrigerator and related equipment will be installed.
- The conceptual design for new instruments will be completed, and long-lead-time procurements will be initiated.
- The neutron-guide designs will be completed.
- The shielding design will be completed.
- A user program will be developed.
- The JINS design will be completed, an RFP will be issued, and a construction contract will be awarded.

After showing a schedule for the reflector replacement and neutron scattering upgrades, Roberto commented on user programs.

Users at HFIR have more than doubled in recent years, but declined 15% in FY 1998 because of reduced reactor availability. User demand greatly exceeds available beam time and support capabilities. First-time users have accounted for more than 20% of all users for the past three years as ORNL has tried to broaden the base of users. Women, minorities, and students each account for more than 15% of the users. Currently, user proposals receive external (e-mail) review and are scheduled year-round. New procedures are being developed to handle the increased demand that is expected to occur with the cold source and other neutron scattering enhancements. The infrastructure proposed to be provided to each user includes:

- An average of one scientific staff member and one technician per instrument;
- An average of one postdoctoral/student per scientific staff member;

- Two administrative persons dedicated to user communication, processing, and support;
- The JINS, which will be available in mid-2000 to provide a one-stop user interface with ORNL, user offices, overnight accommodations, and an outreach program that includes workshops;
- Additional user offices and sample preparation laboratories at HFIR;
- A formal user program with independent proposal reviews administered through the JINS; and
- Additional financial support for students, first-time users, and visitor programs.

The Neutron User Support Facility has been completed with 20 modular offices; the JINS is on schedule for a 1999 construction start; preparations have been completed for establishing a Spallation Neutron Source (SNS)/HFIR users group; external advisory committees are involved in key projects; instrument development teams have been formed for the new cold instruments; and broad community involvement has been fostered through workshops, newsletters and presentations. Relative to the SNS, Sinha asked if the instrument development teams would function like a participating research team (PRT) and was told no, the teams will come together to design the instruments, but the facility will own and operate them. Russell asked about staffing and was told that the staff will be more than doubled to accommodate a tripling in the number of users.

The JINS will be an $8 million facility funded by the State of Tennessee and will constitute a one-stop HFIR/SNS user support facility for badging, office space, housing, telecommunications, and computer support. It will be an intellectual center for the neutron sciences, with conference facilities, workshops, summer schools, visiting programs, and educational and industrial outreach. It will serve as a gateway to HFIR/SNS for students, faculty, and users from universities, industry, and government laboratories and will be a focus for regional cooperation in the neutron sciences. The University of Tennessee will provide ten new faculty positions during the next five years. A site between the SNS and HFIR has been selected, and construction will start in 1999. Richmond asked if the Tennessee money was for staff and was told it is all for facilities. Batterman asked what "joint" meant in this context; Roberto said it referred to a partnership between regional universities and ORNL. Garrison asked if The University of Tennessee would get preferential treatment and was told that everyone would be on an equal footing.

The HFIR neutron scattering enhancements will complement the SNS, particularly for cold-neutron research and "single-channel" experiments. The enhanced HFIR will have 14 state-of-the-art neutron scattering instruments while preserving world-class capabilities in isotope production, materials irradiation, and activation analysis. Its cold source performance will be comparable to the world's best, with a thermal-neutron intensity that is two to three times the current world's best. These capabilities will be implemented in 2000–2001, providing a driving force for continued growth of the U.S. neutron scattering community. The combination of SNS and the enhanced HFIR will help restore U.S. leadership in neutron science.

Roberto summarized his talk by saying that
- All projects are on schedule for beginning the beryllium changeout in April 2000;
- Performance estimates are on target;

- A detailed cost, schedule, and resource-loading model is in place;
- Major procurements are on schedule;
- Advisory committees and instrument-development teams are in place; and
- The first users meeting is scheduled for November 9–11, 1998.

Sinha asked if the user numbers just counted each person or industrial institution once and whether the 50 ORNL users listed were from all the divisions of ORNL or just the operating division. The answer to the first question was yes and to the second, all divisions, with about 40% of the beam time being used by in-house users.

Russell asked what the operating budget was. Roberto responded, $25 million, but $2-3 million more each year would be helpful. Russell asked what those additional funds would be used for; the response was to support needed infrastructure improvements. Russell asked if the HFIR's time frame meshed with that of the SNS. Roberto said that is why they have established a formal work-tracking model to coordinate HFIR and SNS needs for resources such as analysts and designers. Russell asked, "When there is a competition, who wins?" Roberto said that it is Bill Appleton's job to make sure that everybody wins. Garrison noted that he had said that 50 people from ORNL used 40% of the time. He restated it as 40% of the neutron scattering time.

Williams asked how underutilized the reactor was. Roberto said that ORNL could fully utilize 100% of the available time with no help from outside users; the problem was not to find users but to broaden the user base. Crow asked how they were going to triple the number of users by only doubling the number of instruments. Roberto pointed out that the small-angle neutron scattering device is a high-throughput instrument serving more users per unit time; plus, the intensity is being tripled for many instruments.

Batterman asked what fraction of the dollars went to neutron scattering. Roberto responded that they counted neutrons, not dollars; beam tubes use one-third of the neutrons, and that will continue. The neutron scattering is funded by the Division of Materials Science. Other users are funded by other divisions. More than $25 million has been put into the facility as capital investment: $12 million for the beryllium reflector, $10 million for the cold source, $2 million for the cold-beam guides, and $2 million for the thermal-beam guides.

Lester asked about the researchers whose proposals for use of the facility were not successful. Roberto said that they allocate 60% of the time that is requested. Rejected proposals are put off in time, and the staff at the laboratory tries to help the applicants strengthen their proposals.

Dehmer asked how they estimated the needed increase in funding. Roberto said they looked at ILL and what their costs were. She asked what the maximum number of users might be. He responded 500.

Richmond declared a 5-minute break. Upon reconvening, **Jack Crow** took the floor to announce that the draft report from the HFIR Review Panel was finalized after the exchange of an enormous number of e-mails and telephone calls following the two-day review in Oak Ridge. He named and thanked the panel and the Oak Ridge personnel for their cooperation and help.

Crow reviewed the history of the HFIR: It was designed and built in the early sixties, achieved criticality in 1965, and operated at 100-MW full power from 1966 to 1986. It was down from 1986 to 1990 and has operated at a full power of 85 MW since then. With the upgrades completed, it is expected to operate at that full power level until 2035. With the upgrades, the HFIR will be competitive with the ILL and other facilities, but will not close the gap in U.S. neutron science.

He reiterated the HFIR upgrade projects detailed earlier by Roberto. He commended the Oak Ridge effort to set up the JINS, which will enhance the neutron scattering community tremendously. However, he pointed out, the review panel raised the issue of how the management of the facility will respond to new research communities that are not now represented among the management (e.g., biological sciences).

He pointed out that the review and the subsequent report were organized around the five questions posed by DOE in the original charges to the HFIR Review Panel:

1. What has been the scientific and technological impact of the High Flux Isotope Reactor during the past decade, and what is it expected to be during the next decade?

HFIR has been a high performer, making significant contributions in materials science; the soft-matter work is in polymers and condensed matter. The biological sciences are absent; this is a weakness that needs to be addressed by ORNL. Much of the materials science research will migrate to the SNS; the biological-sciences research will remain. In isotope production, reliability is a problem; the facilities need to be available on a regular basis. An income stream from isotope customers helps pay for the facility, and it is important to protect that income stream.

Tirrell asked if biologists are supported at the facility. Crow said that biologists need an instrument person on the staff; ORNL recognizes the need to improve these services. Sinha commented that neutron scattering is a niche activity in biology and asked if a huge increase in biological users is expected. Crow said that there is almost no service to this community now, that the review panel was concerned with this lack, and that the HFBR was no longer available. Batterman said that biology is an active area but that he was not convinced that the biological community has that great a need for neutrons. Crow asked other committee members to respond to this comment. Michael Rowe pointed out that they had a biologist on the committee (Jill Trewhella) who said that there would not be a ground swell of use but that some research will *require* such a facility. She expected that about 25% of the machine time could be used for biological research. Robert Briber said that small-angle scattering will be where the growth occurs and that it will not migrate to the SNS. John Stringer said HFIR is looking at more small-angle scattering and for an improvement in the S/N ratio.

Crow continued, stating that the current user communities that HFIR serves are in neutron scattering, transplutonium production, and isotope production. He pointed out that universities use about one-third of the time on the machine and have recently dropped off. Russell asked if most of the loss in users occurred in foreign users. Crow said that a drop-off in university users has occurred because of the simultaneous unavailability of both the HFBR and the HFIR; more

than just market forces are coming into play here. Russell asked where the users have gone. Crow said some had gone to the National Institute of Standards and Technology (NIST), some Japanese research had evaporated, and some had gone to Europe (e.g., ILL). Russell asked why, and Crow responded that you do not plan a research project around a facility that is having problems.

Crow continued that user satisfaction is generally high, although users have had software and other technical problems in transporting data home to analyze it. Software is needed to turn data into science.

2. What is the level of user demand for the reactor, and how is it changing? How does the current shutdown of the High-Flux Beam Reactor at Brookhaven National Laboratory affect the user demand at HFIR?

User demand has been difficult to judge because of the availability problems in the past few years. The user program has historically been driven by collaborative research projects. This practice has changed and should have begun over three years ago with their self assessment. The question should have come up in 1990 and only now in 1998 is a user's group being formed.

Russell asked how user demand was judged. Briber said they met with a limited sample of users; reliability was the major concern. Garrison asked how the users were selected. James Ball answered that the users were the ones that happened to be on-site at the time, running experiments. Leone asked what type of outreach activities were being carried out. Crow responded that ORNL has pursued some outreach, and you see high-quality research being done and a high utilization rate; but when you realize that NIST has the only other facility friendly to biosciences, you would expect to see more representation from those sciences in the user advisory groups at ORNL. Operating in a collaborative mode provides some benefits, but it should only be a part of the users' input.

Richmond said if you put money into making a facility more reliable, that means taking funds away from other needs, and asked whether the panel got any idea of how high a priority ORNL put on upgrading reliability. Crow said that they did not and were not charged with delving into budgetary concerns, but reliability enhancement has to be the top priority. The HFBR was going off-line at the same time that the HFIR was having availability problems, so work that might have shifted from BNL to ORNL did not occur. Russell asked if the HFIR upgrade would relieve the overload at NIST. Crow responded that a different suite of instruments existed there, but certainly some of the work at NIST can be done at the upgraded HFIR.

3. Is the full range of user issues currently being adequately addressed with respect to the current operating schedule and within the facilities available?

The panel felt that the attitude toward users had to be changed. The plan presented at the panel's meeting with ORNL personnel was inadequate. However, since that review, the user program has been thought out much more fully (referring to the planned SNS-HFIR Neutron Users Meeting and the JINS plans that were described by Roberto). Garrison said that the comments seem to be the same ones that we heard with the Advanced Light Source and other user facilities

and asked why the laboratories do not look at what others are doing and do that. Crow responded that other influences come into play. We are seeing a large number of changes not only in facilities but also in the philosophy of how these facilities are to be operated, and large sums of money are on the table. Russell asked if ORNL had a user group in place. Crow responded that when the long shutdown occurred beginning in 1986, the National Science Foundation (NSF) pulled their support of small angle neutron scattering, and the user group dissipated. He went on to say that the panel is interested in the integration of the HFIR and SNS users operations. This topic is being addressed at the SNS Instrumentation Workshop and Oak Ridge Neutron Users Meeting in November.

4. From the user perspective, how good are the availability, dependability, and reliability of the reactor and user-support infrastructures, including critical instrumentation packages and support personnel?

The reliability during the past two years has not been tolerable or able to maintain a world-class facility. Then there were the shutdown, self-assessment, and management reorganization. Reliability must be the top priority in repairing relations with users and customers. The reliability problems are caused mainly by aging equipment.

5. What is the relation of the HFIR to other activities at ORNL [e.g., the planned Spallation Neutron Source (SNS) and the Radiochemical Engineering Development Center (REDC)]?

The upgrade will bring in a suite of instruments that will be competitive with other sources, although the S/N ratio problem still needs to be addressed. Some work will migrate to the SNS, but a significant portion of capabilities will stay at the HFIR. This process of dividing the work needs coordination, includes the hiring of additional staff, requires the identification of research opportunities, etc.

The panel came to five critical recommendations for ORNL (here ordered in greater to lesser priority):

- Develop a plan to address the long-term reliability of the HFIR that identifies the amount and source of the necessary resources.
- Develop a coherent vision of the expected outcome of the ongoing upgrades and develop and implement a management plan to reach that goal.
- Develop a plan for a high-quality user program at the upgraded HFIR that is *tightly coordinated* with development of the user program at the SNS.
- Consult the relevant neutron scattering communities and develop a staffing plan for increased utilization that broadens the existing science program.
- Work closely with the irradiation and isotope communities to ensure that their needs are met to the maximum possible extent.

Leone asked where the users have gone when the HFIR has not been available. Crow said Europe, NIST, etc. Leone understood the companies to say that they got better service by going to Europe and asked if the report reflected that. Crow said no, it did not but the panel recognized that even this small user community should be better represented in the discussions of future operations. Smalley asked what neutron scattering work could be done at the HFIR that could

not be done elsewhere. Crow responded that small-angle scattering will be a dominant center of gravity after the HFIR upgrade. Rowe commented that, if background and other problems can be solved, a lot of experiments requiring high fluxes and/or long durations will require the HFIR. Smalley asked how much the NIST reactor ran, and Crow said 24 hours a day, 250 days a year, about the same 70% that HFIR aims for.

Meyers asked whose responsibility it was to develop these user groups. Crow said it was the responsibility of the facility. The JINS is just a building; there has to be a plan, a set of goals, and a vision on using the facility and expanding outreach to potential users. Roberto said that the agreement with The University of Tennessee places that responsibility squarely on ORNL.

To respond to several comments about the perceptions of the "good old boy network" at HFIR, Horton said this was a concern years ago, but the younger staff who have been hired reflect both women and minorities. Horton said that she was also proud of the diversity indicated by the Laboratory's funding of new research programs in emerging technologies (e.g., residual stress analysis) that has been important in attracting new industrial partners. Contrary to some comments made earlier, the existing condensed matter physics neutron scattering community was selfless in the "sharing of neutrons" and fully supported the development of new scientific directions. Russell commented that old boys do not have to be old or boys; the problem is the perception of accessibility by outsiders. Batterman said that the old-boys network gave you good science but not in an equitable way; that is what is wrong with that network. We must change and build upon the strengths. Crow said that ORNL is doing just that.

Dehmer pointed out that the reactor was not built as a user facility. It was built for ORNL and its collaborators. Many of the issues we are talking about have come up because we are trying to make a transition to a user facility.

Richmond asked for a vote accepting the report and its recommendations. The committee unanimously accepted the report and recommendations. A break for lunch was declared at 12:28 p.m.

Richmond called the committee back into session at 1:36 p.m. and introduced **Stephen Leone**, who has been asked to head the BESAC Panel on Novel Coherent Light Sources. He said that the charge was broader than the so-called "fourth-generation light sources" (free electron lasers). In response to this, DOE agreed that the group should be called the Panel on Novel Coherent Light Sources. The panel has been asked to address what new DOE science may become accessible by new light sources based on advanced concepts, including synchrotron-based methods, free-electron lasers, table-top laser systems, and undiscovered methods. This panel may be the last opportunity to look across all these systems and be able to make recommendations on a prudent course of action for BES.

The panel will ask laboratories to present their science ideas and light-source concepts at a meeting on January 21, 1999. Sources based on table-top methods will be included along with accelerator-physics methods like free-neutron lasers. Presentations will be given by several people outside the laboratories. Leone said that what the panel will be looking for are new light outputs and what characteristics might be achieved in coherence, wavelength, power, time

duration, etc. The panel will also ask in what time frame such source development could be realized, what research would be needed for development, and what new DOE and non-DOE science could be achieved if these sources came about.

He listed the current panel composition along with the positions that are yet to be filled. He said that the next steps are to fill out the panel, send a letter to the laboratories to tell them what we are trying to accomplish, and to solicit speakers from outside the laboratories.

Horton asked if the representatives from the laboratories would be members of the panel. Leone replied, no. She also asked why there were three table-top-laser experts on the panel. Leone responded that he felt that the panel would be overwhelmed with input from the accelerator representatives, so he tried to balance the constituencies. Lester asked what is different about this from previous, similar assessments. Leone responded that the other assessments did not consider DOE's needs and perspectives. This panel will take those other panels' suggestions into consideration and apply them to the needs of and opportunities for DOE. In response to a question from Garrison, Leone responded that the panel is supposed to be looking at the science, not the construction of light sources. We need to see what concepts and possibilities exist. Batterman said that this arrangement seemed unbalanced to him and asked why there are not more accelerator people on the panel. Leone said the laboratories will be invited to cover all aspects of the science that can be acheived with lasers as well as accelerator concepts. The panel will bring in some outside representatives to cover other laser concepts. He then listed the laboratories to be invited; no foreign laboratories were included.

Sinha asked if this committee will plan a course of action for DOE or just identify interesting fields of science. Leone responded that the panel will make prudent recommendations; typically, it will get visions of what is possible today, not what may be possible 8 to 10 years from now. Sinha followed up, asking if he expected to identify what kind of facility will be needed. Leone responded that the Panel could only recommend some prudent ways to spend some seed money now.

Batterman said that a strong case has been made to go on to a new generation of light source. The Birgeneau committee said that we need to determine which direction to go, not whether there is interesting science to be done. Leone said that the charge letter does not state that. This committee does not intend to select a specific path of inquiry. Thomas read the charge letter. The request was broader than the interests considered by the Birgeneau committee. Thomas said that he did not believe that the science question has been answered. Dehmer said that she agreed; in some cases, conventional light sources compete well with free-electron lasers. Batterman said that he thought that the science had already been explored and that the panel should meet to get to the decision of how we should accomplish that science. Dehmer said that the major dilemma is where you put limited resources. When you are talking about something like free-electron lasers, the resources are very limited, about $3 million. Batterman said that when you say that something is going to be three to four orders of magnitude more powerful than what we have now, he gets excited and wants to know how to get to that point. Russell said the Birgeneau report recognized the science was there, but the case to justify pursuing it was not made. The characteristics of the sources proposed were not discussed.

Leone commented that he was looking for a few more people who would look at this complicated task and lend new insights about it. Richmond stressed the charges made in the letter and said that we now need personnel to address these issues. She opened the discussion to public comment. Bev Hartline of the Office of Science and Technology Policy (OSTP) commented that the panel should have people with machine and technology experience so it can do the second part of its charge. Sinha noted that we need someone with experience in the technology of x-ray optics. (In discussion on the next day, Shen suggested that the senior people on the Leone Panel might benefit from the presence of some younger, junior researchers among the members.)

Richmond then introduced **Mike Knotek** to speak on the Strategic Simulation Initiative (SSI). He began by noting that the information from his presentation to this committee in July is available on the Energy Research (ER) website (http://www.er.doe.gov/ssi/ssisum.htm). Since that presentation, a meeting was held with the NSF, and the summary report of that workshop is also on the ER website (http://www.er.doe.gov/ssi/LangerReport.html). The DOE-NSF workshop enthusiastically supported the SSI and made seven recommendations on how to promote and implement the initiative. A larger impact, however, was made by the interim report of the President's Information Technology Advisory Committee (PITAC), which is also available on the web (http://www.ccic.gov/ac/interim/). This report calls for the doubling of the funding for research on high-performance computing (a billion dollars more per year), major research in software, the development of a scaleable information infrastructure, major investments in high-end computing, the application of teraflop computing to real-world problems by 2010, and the addressing of the social and economic issues related to technology adoption and diffusion. These recommendations are being followed up by the OSTP, the Federal High-End Computing and Computation Program, and the Economic Council. The committee recommended that the NSF be designated as the lead federal agency for coordinating information-technology research. The Department of Energy is working in partnership with several other agencies, particularly the NSF. The National Institutes of Health (NIH) are taking a hard look at their computing; they will be a big force in this initiative. Another joint DOE-NSF workshop is expected to plan how to progress in this area.

Sinha asked what part of DOE will carry the ball in this program. Knotek said that all of ER is involved, but how we will bundle the management is still unknown. Something will have to pull all of this together.

Knotek then introduced **Bill Kirchoff**, manager of BES's Chemical Physics Program, to summarize the details of the SSI. Kirchoff started with a timeline of activities for the current calendar year. In January and February, the first workshops were held, covering materials and geophysics, geochemistry, large quantum-mechanical systems, nonlinear complex phenomena, simulation and modeling, data analysis and management, and applied mathematics and computer-science techniques. Out of these workshops came a very long list of research topics that were subsequently reviewed for relevance and potential impact. In March, the applications that would be part of DOE's initiative were selected: climate prediction, combustion, and basic science (including fusion energy, structural genomics, materials, high-energy physics, and subsurface transport). From April to July, a series of directed workshops was held on each of these selected topics, resulting in a number of white papers outlining the scientific challenges of

each and the approaches to be taken. On June 5, the President featured the initiative in his commencement address at the Massachusetts Institute of Technology (MIT). On July 30 and 31, the DOE-NSF workshop was held. In August, PITAC issued its interim report to the President. From September to December, the federal initiative is being developed.

Kirchoff then turned his attention to combustion simulation and modeling. Much of the BES Chemical Sciences research in chemical physics is being done to advance the predictive capability for combustion processes. To put the problem in perspective, he described a simple but elegant experiment involving methane combustion that challenges the traditional models of the combustion process. He pointed out that running the modeling simulation of this highly simplified experiment takes six to eight weeks on a large computer. The simulation, based on a reaction mechanism of 176 reactions (and their reverse reactions), did not match the experiment.. At current run speeds, it is impossible to make iterative calculations to determine which one (or ones) of these reactions needs to be fine-tuned.

Several scientific fields contribute to combustion science. Theoretical methods for calculating reaction rate constants and other aspects of combustion chemistry are broadly applicable to all chemistry. Because of its complexity, combustion was broken up into manageable regimes at the atomistic, fine-continuum, and device levels. A workshop was held on each of these levels. The plan is to break each of these levels down into packets and to model each packet. To use an analogy from theoretical chemistry, the approach is similar to the Born-Oppenheimer approximation. The workshops held from April to July addressed the problems of simulating and modeling combustion. They resulted in a draft plan of 150 pages, which was peer reviewed in July. The revised plan, based on the review recommendations, will appear soon.

Kirchoff listed the recommendations of the PITAC interim report and pointed out that a high degree of collaboration among the laboratories will be needed to carry this initiative to fruition. Garrison asked if the problem would be addressed at the laboratories, and Kirchoff replied that two RFPs would be issued: one to the laboratories and one to the broader scientific community. Sinha asked if the automobile industries are involved. Kirchoff answered that they were. One previous program was the diesel collaboratory; from that grew a diesel CRADA (cooperative research and development agreement) with Cummins, Caterpiller, Sandia National Laboratories, Los Alamos National Laboratory (LANL), and Lawrence Livermore National Laboratory. The DOE Office of Transportation Technologies in the Office of Energy Efficiency and Renewable Energy, the ER Office of Computation and Technology Research, and BES expanded that into diesel combustion modeling program, and the number of industries and educational institutions was expanded. The computational resources and the basic science involved are beyond industry's capabilities. Garrison asked whether there will be a central place to apply for funding. He said that there will be interagency coordination, but agencies will fund specific projects individually.

He then introduced **Daniel Hitchcock** of the DOE's Office of Computational and Technology Research. Hitchcock reiterated that if DOE's SSI was funded, the funding would be split among climate systems, combustion, and basic sciences. At this level, computing is much more complex and provides tremendous amounts of data that require analysis. Therefore, portions of each of these three allocations would go toward (1) computer science and enabling technology

(CSET) and (2) computing and communications facilities. He noted that it is important to build this software to serve all applications because you cannot afford to build it a second time. The SSI will come with a number of challenges:

- Teraflop computers will be hard to use.
- Current approaches to data management, analysis, and visualization do not scale to the future; for example, disk drives are getting bigger, but transfer rates are staying the same; a 40-teraflop machine requires a teraflop/second transfer rate at the machine level.
- Ways to enable remote collaboration and use of these resources are needed.
- Many current algorithms scale poorly with problem size.
- Applications need stable, engineered tools; application software must be modularized.
- The CSET must be a balanced program with research, development, and deployment.
- Software development must be geared to specific components.
- The software developed for the SSI must not be isolated from that serving the midrange computers; it is too expensive.

The CSET program would develop

- algorithms, models, methods, and libraries;
- problem-solving environments and tools;
- distributed computing and collaboration technology; and
- visualization and data-management systems.

Many of these have hope for developing a good solution once and then using it in all applications.

The SSI will be built on the experience gained from planning and beginning to execute the Accelerated Strategic Computing Initiative (ASCI), which was developed for the stewardship of the nation's stockpile of nuclear weapons. In certain core areas, the SSI will codevelop software technology with ASCI to ensure that these technologies can be effectively deployed to strategic-simulation applications. In a number of areas, the SSI will have to significantly extend ASCI technologies or develop different technologies.

He then reviewed the PITAC recommendations and showed that the SSI would address virtually all of them.

Thomas commented that, upon first consideration, transitioning to the new level of computers seems like it should be straightforward, but computing at this level is like computing was in 1974. Systems are getting much more complicated. Getting high-level code to run and work will be difficult; most of the old algorithms will have to be reengineered from scratch.

A break was declared by Richmond at 3:30 p.m. She called the committee back to order at 3:50 p.m. and introduced **Robert Marianelli**, to speak about OSTP, its structure and missions, and the policy-making process. He started by pointing out themes that recur in presidential and vice-presidential speeches:

- Technology and the underlying science are responsible for more than one-half of the productivity increases during the past 50 years.

- The sciences are interdependent; for example, the biomedical sciences depend on natural science, mathematics, and engineering.

He described the structure of OSTP, which, with a staff of 60, is not a large organization. It is part of the Executive Office of the President, and its directors are confirmed by the Senate. It advises the President on policy matters related to science and technology and coordinates interagency activities. Its programs are guided by a series of principles that include the use of peer review; forging partnerships with industry, universities, or states; employment of realistic and objective measures of progress and performance; improving interactions with state and local governments; enhancing the professional capacity of the workforce; and promoting international cooperation.

He showed a chart that indicated increased investments in civilian R&D, basic research, applied research, and R&D infrastructure in the FY 1999 and 2003 budgets. Further analysis of these figures showed that the currently proposed budgets and budget resolutions provide increases for NIH, but provide only level or decreasing levels of funding (unadjusted for inflation) for non-NIH civilian R&D. Moreover, the FY 1999 budget postulated revenues obtained through tobacco legislation to pay for some research, and that funding source did not materialize. So, for R&D to go forward, new money has to be found, or an offset has to be made. A table detailing changes in federal investment in scientific research showed an increase of $1.934 billion for NIH, $243 million for NSF, and $215 million for DOE (of which $130 million is for the SNS).

He posed the question, "How is policy made?" He noted that the President stated in his commencement address at MIT that he would call for funding of computing and communications research and had directed the head of OSTP to draw up a plan for such funding. One of the staffers in the president's office had put this statement into the speech. The President approved it and it became policy. What happens to this idea now depends on the availability of resources. The effort to establish a major initiative does not end when it goes to the Office of Management and Budget (OMB); it *starts* when the initiative goes to OMB.

He pointed out that current minorities will increase as part of the population. As a result, the participation of the current minorities in science and technology must increase if we are to maintain a high standard of living. As a result, OSTP has convened an interagency working group on the 21st century workforce to examine the demographic changes and the intrinsic values of diversity. It will systematically review federal programs relevant to increasing participation, see where opportunities exist to enhance participation by minorities, and propose programs to accomplish such enhancement.

Commenting on user facilities, he stated that:

- The administration favors merit-based access to scientific resources.
- Substantial financial and intellectual investments are needed to construct and support beam lines and ancillary equipment.
- Public availability has to be weighed against access for groups that make substantial investments in the facilities.
- These facilities should undergo routine analysis.
- A working group including NIH, NSF, DOE, and NIST has been convened to consider issues related to synchrotron use for structural biology.

He commented on the need to communicate to the general populace the promise of and need for science. Horton called his attention to a book, *Worlds Apart*, which talks about the disjunction between science and the reporting of science to the general public. Williams pointed out that, if you cannot communicate a concept to people in terms of the first order, you will lose them when you go on to the second and third orders.

Smalley asked if Marianelli heard a call from the nation for new energy resources and clean technologies. He responded that he understood that this was in terms of the environment and that energy technologies are an important part of those concerns.

The discussion was opened to the public, and Mark Crawford of *New Technology Week* asked Marianelli if he saw the administration providing leadership for school administration. He responded that it was not an area he was knowledgeable about. He did comment that a recent report said that in student testing at Shaker Heights, the minorities did not do as well as the rest of the population, and it was not understood why. Facts such as these make it clear we need to engage the whole of society in preparing the workforce for the future. Mentoring is an important component of preparing that workforce and both schools and families are important parts of this effort. He pointed out that at times well intentioned efforts go awry. For example, the funding of DOE education programs disappeared, and programs with educational applications are now struggling.

There being no other questions, Richmond adjourned the meeting at 4:41 p.m.

October 27, 1998

Richmond called the meeting to order at 8:32 a.m. and introduced **Patricia Dehmer** to review budgetary developments. Dehmer reported that, with the FY 1999 budget, funding of the core research is essentially flat; the increases and decreases are in the special programs: the SNS went from $23 million in FY 1998 to $157 million in FY 1999, the Climate Change Technology Initiative went from $0 to $16 million, construction of the Combustion Research Facility went from $7 million to $4 million, and user-facilities operation went up almost $22 million (as a direct result of the compelling reasons for improving the light sources put forward in the Birgeneau report).

She showed the amounts actually appropriated for each office of Energy Research. The largest increases from FY 1998 to FY 1999 were for Biological and Environmental Research. High-Energy Physics, Nuclear Physics, and Fusion Energy Science had modest gains. Basic Energy Sciences showed a large gain, but showed a modest decrease when the SNS construction was accounted for. Computational and Technology Research showed a large decrease because of the reduction in funding for the next-generation Internet. The figures shown would be decreased by general reductions that are applied to each division. She cautioned that the FY 2000 budget has not yet been revealed by the White House and that DOE cannot issue mortgages until it sees what directions are contained in that budgeting directive.

Russell asked if she could give an update on the SNS. She said the SNS is progressing well and that receiving the funding for FY 1999 was very significant. The teams are in place at all the laboratories, a project manager has been selected by LANL, and an NSF-DOE workshop in Knoxville in November will look at neutron scattering opportunities. She expressed great optimism for the project. Russell asked about the environmental impact statement (EIS) for the SNS and that for the HFBR. She said that the draft EIS for the SNS will be issued by mid-December and that the decision on the restart of the HFBR would be made by next June after the EIS for that facility is completed.

Charles Shank, Director of Lawrence Berkeley National Laboratory (LBNL), was then asked to conduct a discussion of the Complex and Collective Phenomena Initiative. He prefaced the session by saying that he hoped to inspire discussion rather than produce an end product, to find ideas on what topics might be addressed if we go forward with this initiative, and to identify what components of science we are trying to bring together. A workshop has tentatively been scheduled for January. The question is, what should be the scope of the workshop? What the workshop comes up with could very well change how we practice biology, physics, environmental sciences, materials science, geophysics, and chemistry. He offered a selection of scientific issues that might reflect the complex systems that were to be discussed: nonequilibrium systems, functional syntheses (predicting structure function), control of entropy, strongly coupled systems, scaling in space and time, and understanding heterogeneous environments. As examples of topics that might be considered, he suggested:

- Dendrimers (very complicated structures) as novel catalysts
- Control of entropy by self-assembling photoactive molecules
- Protein biosynthesis of new types of molecules
- Functional genomics with unnatural organisms (We have 20 amino acids; why not 21? If we created amino acid no. 21, we could make unnatural organisms. Some 60 additional amino acids have been identified in the California genetic code.)
- Phenomena beyond independent particle approximation (e.g., in cuprate superconductors)
- Semiconductor nanocrystallites: building blocks for quantum-dot structures
- Chemical heterogeneity in soil organic molecules

The needs at hand are to set up an organizing committee, select five or six areas, and have experts in those five or six areas address a workshop.

Smalley asked if Shank could postulate a razor that would separate complex from noncomplex research. Shank said there is complexity in all science. He would like to limit the effort to

looking at areas in which complexity is a barrier to new understanding. Smalley suggested "where some new property is not apparent because of the complexity." "Exactly," said Shank. We might need new ways of looking at problems that depart from traditional ways of approaching those problems. Smalley said he was willing to bet that every BES program could be seen to possess such properties. Dehmer said it goes beyond BES to all of ER.

Shen suggested that the relationship between diversity and universality may be a distinguishing characteristic. As scientists, he said, we look at vast amounts of data and search for patterns in those data, patterns that reflect the operation of some underlying process or law. Physics has collapsed its knowledge to several universalities, but can we find universality or organizing principles in such complex fields as biology? Shank agreed; he said we should be looking for a simpler, organizing principle to any complex system.

Richmond asked how many participants did he envision taking part in the workshop and what time frame he thought it would follow. He said he hoped to put together an organizing committee of 10 to 15 people in the next week or two. They would meet by telephone and identify five or six topics for discussion and a speaker for each topic by mid-November. These presentations would then be made at the workshop in January at LBNL. Richmond was concerned that important discussions would be occurring in the phone conversations and that this critical brainstorming may be subject to limitations in discussion. Shank countered that getting 75 people together with no structure would be very difficult to get something out of. Horton said that this topic has been discussed at the ER Strategic Planning Meeting and that each field thinks that what it is doing is the ultimate in complexity. Care must be taken that one field does not dominate the limited number of topics discussed.

Shank said that today's deliberations should focus on Smalley's and Shen's comments and suggestions. We will have to impose some constraints and be careful in selecting these constraints. We have to start with some selection of people, and that selection of people has to include every element.

Sinha said that he was not sure that high-energy physics fell under the definition of complexity put forward. It seemed that nuclear physics might, but not high-energy. Thomas said that you would not have a proton without the collective behavior of quarks.

Shen said that he understood that a similar workshop was to be held at LANL this winter and wondered if there was any connection. Shank said that this workshop was for LANL only, and that he hoped to learn from that experience. He asked how BESAC would advise him to select the next step. Richmond suggested that he use a broad selection of the best people but avoid the chaos of a large collection of people. She said that the selection of people for the dialogue is very critical.

Smalley said that "complexity" does not express the exciting concept here. What is exciting is emergent phenomena, but that is not in the title. He wondered what scale we are looking at. He observed that most of the topics that Shank had put out as examples were on the scale of thousands or millions of molecules. We should therefore concentrate on the nanometer scale. Adding more amino acids is a great example. He thought that some portion of this effort should

be focused on "nanotechnology." Shank said that the nanometer scale *is* fascinating, but geophysicists talk in terms of hundreds of meters and thousands of years (in tectonics, for example), and this additional topic should come out in the workshop.

Williams commented that we have to pick something that can be done in a finite time with finite dollars. Shen said that what we are looking for is a scaling property, a principle that would allow going from smaller systems to larger systems. We need to look for systematic changes as we go from scale to scale. Russell said that the same problem cropped up in materials, a problem that went from the lightwave scale to the molecular. The approach that was taken was to go from the general to how this would affect day-to-day life.

Lester suggested that the selection of overriding themes be postponed beyond January. He said that the selection of such important topics on such a short timeline is worrisome. Shank said that he had the same concerns; if we get down into the nuts and bolts too quickly, we could lose credibility. Horton asked if he had considered having a January meeting to identify various disciplines' concerns and interests and then having a follow-up meeting of the 15-member panel to consider the possibilities put forward. Shank said that the true challenge is getting the right thinking process that goes beyond a single discipline, and that property would obtain no matter how we organized their meetings. He looks upon the organizing committee as a catalyst, with the report being written by the heads of the five breakout groups. Williams interjected that they must have some organizing theme and some limiting scale. Shank stated that the challenge is quite clear: we started with something with very few constraints; the community must bring the constraints. He said if the committee could offer any guidance, he would be very glad to have it. In the end, the initiative will be owned by a limited number of areas that have emergent phenomena and will go forward from there.

Dehmer pointed out that we are looking forward 20 years, not to next year. We want to inspire people for the future using the glimpses that we have today. One of the themes must be to think that way. We want to challenge lawmakers to see that there is a *reason* to put money into scientific research and development. Shen said maybe we should start out in a disparate manner and see if there is some commonality revealed in the first workshop. Horton suggested a cross of the two: listing the technologies that will be important in the next 20 years and then having the panel determine the ones that will garner buy-in from across the ER structure and using that as the final input into the summary of possible directions in this field. Richmond ended the discussion and thanked Shank for his input.

Richmond then announced that Martha Krebs is asking BESAC to review the electron-beam microcharacterization centers. She distributed the charge letter and introduced **Iran Thomas** to talk about the assignment. He pointed out that BES supports four microcharacterization centers, one each at Argonne National Laboratory (ANL), LBNL, ORNL, and the University of Illinois. Unlike our other user facilities, these do not have large operating budgets. For example, the University of Illinois facility charges fees to their users to cover at least a part of their operating costs. The Oak Ridge Institute for Science and Education (ORISE) is a partner in the ORNL program and provides limited travel funds for students and faculty. Several techniques are available at each of these centers. These centers are almost entirely dedicated to materials science. The NIH operates other electron microscopes that are devoted to the biological

sciences. In 1996, the DOE electron beam microcharacterization centers served almost 1000 users from academia and industry. He distributed a handout that detailed the suites of instruments at each site.

He said that it has been more than 10 years since BES evaluated these centers and would like to have an assessment of:

- the scientific and technological impact of these centers during the past decade,
- their expected impact during the coming decade,
- the user demand and how it is expected to change,
- the special needs the centers serve,
- the appropriateness of their visions and whether their visions complement each other, and
- the opportunities for improving the techniques practiced at the centers.

Batterman commented that there is dissatisfaction at the University of Arizona's facility. Thomas noted that the Arizona effort is funded by the NSF and that individuals, not a center, are funded. The NSF and the NIH are currently considering what their roles should be in supporting such research. For the DOE centers, funding has not been provided to keep these facilities at the state of the art and BES would like to know how far from the state of the art we are.

Horton commented that she was concerned that the charge letter indicates that the panel would not visit the facilities. She thought there would be great value added by site visits by at least subgroups of the panel. Dehmer responded that this would be considered when the person to head the panel is identified and they review the charge with that person.

Richmond asked if there was any old business. When the suggestion met no debate, Richmond turned to new business: The next BESAC meeting will be February 24-25, 1999, in Gaithersburg. The meeting after that will be at the end of July or in the beginning of August. She opened the floor to public comment; there being none, she adjourned the meeting at 10:20 a.m.

F. M. O'Hara, Jr. 11/20/98
revision by L. L. Horton, 11/25/98, 12/11/98