Minutes for the
Basic Energy Sciences Advisory Committee Meeting
October 20-21, 2003
Double Tree Hotel, Rockville, Maryland

BESAC members present:

Nora Berrah
Philip Bucksbaum
Sue Clarke
Peter Cummings
George Flynn (Monday only)
Bruce Gates
Laura Greene
John Hemminger, Chairman
Anthony Johnson (Tuesday only)
Kate Kirby
Walter Kohn
Gabrielle Long
William McCurdy, Jr.
Daniel Morse
Martin Moskovits
Ward Plummer
John Richards
Samuel Stupp (Monday only)
Kathleen Taylor
Stanley Williams

BESAC members absent:

Mostafa El-Sayed
Eric Isaacs
Richard Smalley
Mary Wirth

Also participating:

Ian Anderson, Director, Experimental Facilities Division, Oak Ridge National Laboratory
Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Thom H. Dunning, Jr., Director, Joint Institute for Computational Sciences, The University of Tennessee and Oak Ridge National Laboratory
John N. Galayda, Linac Coherent Light Source Project Director, Stanford Linear Accelerator Center
Daniel Hitchcock, Senior Technical Advisor, Office of Advanced Scientific Computing Research, USDOE
Keith Hodgson, Director, Stanford Synchrotron Radiation Laboratory, Stanford University
Harriet Kung, Office of Basic Energy Sciences, USDOE
Alan Laub, Director, SciDAC, ASCR, USDOE
Raymond Orbach, Director, Office of Science, USDOE
Walter Stevens, Office of Basic Energy Sciences, USDOE

Monday, October 20, 2003
Morning Session

Chairman **John Hemminger** called the meeting to order at 8:20 a.m. and asked each Committee member to introduce himself or herself. He introduced **Patricia Dehmer**, Director of the Office of Basic Energy Sciences (BES), to speak about the Office and its operation.

She reviewed the current status of the FY04 budget for BES. The House markup version is $8 million more than requested in the President’s request; all of which is for facility operations. The Senate markup is at the President’s request. The budget is awaiting a House-Senate conference and then an appropriation bill needs to be passed. The Department is operating under a continuing resolution until October 31, 2003; this means that it can expend funds at the FY03 level but can make no new starts. No new starts means that facilities under construction will be impacted. Increases in construction funds or R&D funds will not be available until new appropriations are passed. Some facilities [like the Spallation Neutron Source (SNS)] are winding down their construction activities, so budgetary needs are less than they were last year; therefore, they will not be impacted. Generally, though, BES is executing the budget very conservatively and awaiting the new appropriations.

The FY05 budget is currently under discussion and is therefore embargoed. The chief financial officer has just put a guidance report up on the Web. That office has submitted the budget requests and is awaiting Executive Office review and comments. This budget cycle is well along its normal path,

The FY06 and beyond budgets are open to discussion. BES will be putting out the unicall for funding requests in about a month; then early planning will begin.

The budget for BES is about $1 billion, of which more than 25% goes toward construction, more than 25% goes toward facility operations, and about 40% goes toward R&D.

OMB requested a philosophical overview of the Office's operations and funding. The response was that the Office responds to five investment drivers:

- Outstanding science
- Scientific user facilities and advanced tools for the nation
- Science that addresses the DOE mission
- Stewardship of DOE-owned research institutions (many facilities are aging)
- Workforce development

Of these drivers, the second, third, and fourth are specific to DOE. The challenge is to maintain balance among these five drivers. When an external influence starts to push one of these drivers (e.g., demanding that some facility operate at 100% of capacity), that action presents a difficulty in maintaining balance with flat funding.

This Committee has produced outstanding reports on basic science and reports that address the DOE mission. The two most recent reports, *A Science-Based Case for Large-Scale Simulation* and *Basic Research Needs for the Hydrogen Economy*, have received enormous attention. Planning and budgeting are now tied together in the budget process, and these reports and plans put BES in a good position.

The surplus has given way to a deficit, and significant international financial obligations now exist. The nation has gone to "gloom-and-doom" budget predictions for discretionary spending in FY05 and beyond (i.e., the same predictions as in most of the recent years). This means that science activities will succeed only if they are compelling; important; nonredundant; well justified; well managed; nationally and internationally coordinated, as appropriate; and supported by the community, the Administration, and the Congress. The Office of Science and Technology Policy (OSTP) and the Office of Management and Budget (OMB) will support only activities that meet all these attributes. It will take a lot of work, considerable luck, and everyone pulling in the same direction to succeed. Nothing should be taken for granted.

The stewardship of DOE-owned research institutions got more discussion at OMB than any other topic. DOE's vision is to have the Office of Science (SC) laboratories be acknowledged by all of their "customers and stakeholders" as indispensable components of the nation's scientific infrastructure, seamlessly integrated with academic and other research institutions. The SC laboratories should be:

- Recognized as world class

- $ The stewards of large-scale science capabilities serving the entire U.S. science community
- $ Hosts to tens of thousands of visitors annually (currently about 20,000)
- $ Innovators of big ideas and research constructs, capitalizing on the capabilities of nonacademic institutions (large machines and lots of mobility)
- $ Intellectual and business partners with academic institutions in long-term, large-scale, transformational science projects requiring a scale, staff, and infrastructure not available at an academic institution
- $ Probably cross-staffed with academic institutions
- $ Leaders in basic and applied energy and environmental research, frequently in collaboration with academic and other research institutions

Two new charges have been put to BESAC:

1. Carry on a Committee of Visitors (COV) review of the activities within the new Scientific User Facilities Division with a report to BESAC at the summer or fall 2004 BESAC meeting
2. Put together a BESAC subcommittee to consider theory, high-end computing, work-station/cluster computing, and algorithm development as they pertain to the research activities of the BES programs.

The subcommittee should identify and assess the major opportunities to advance the research supported by the Basic Energy Sciences program through high-end computing (HEC) and through conventional (workstation and cluster) computing. It should summarize the recent past and projected future scientific impacts of each of these types of computing. It should identify research areas supported by the Basic Energy Sciences program that are now using HEC, are ready to use HEC, or that might benefit from HEC in the near future. And it should assess the challenges and needs for the use of HEC (e.g., the development of theory, mathematical algorithms, system software, and hardware architectures; the availability of and access to HEC machines and the customization of HEC machines; and the funding requirements).

A COV assessed the Division of Materials Sciences and Engineering and identified several issues. One of the conclusions of the first BES COV (for chemistry programs) was that there was a need for the standardization of the documentation of decisions, processes, reviews, etc. The recent COV was pleased to observe that the implementation of this recommendation was well along the road to completion. Its specific recommendations for enhancements to the documentation are:

1. A time line/document page should be developed that would be affixed to the inside cover of every project folder. This page could contain a checklist with all critical milestones in the proposal process with space to enter dates and comments. [This has since been done.]
2. The use of mail peer reviews is an integral part of the decision-making process for BES. The COV stated that the review process would be improved if a reviewer "report form" were developed to help ensure that the reviewer provides as much appropriate information as possible. [BES has struggled with this task, but has not yet figured out how to accomplish it.]

The COV found that the Office of Science information management system is ineffective in many ways. The COV and the Office would like to see the following specific information collected and available:

- $ Reliable statistics on longevity of projects for all the programs
- $ Reliable statistics on diversity of principal investigators (PIs) and researchers funded by the programs
- $ A complete listing of proposals received by each program during the 3-year period of evaluation, including information on outcome (fund/not fund), reviewers used, previous

funding history of the PI, etc.

- Data on length of time from submission to funding decision
- Reviewer database

The proposal-review process would be more valuable if verbatim copies of the text of the reviews were transmitted to the PIs in all cases in such a manner as to keep confidential the identity of the reviewer.

A set of “conflict of interest” guidelines should be included with each review solicitation. PIs should be asked to supply a list of mentors, former students, postdoctoral associates, and collaborators for the previous 5 years as part of the proposal submission.

Consideration should be given to a more widespread use of contractor’s meetings. Contractor’s meetings provide a number of benefits in addition to allowing the program manager to remain up to date on project progress.

While it might require difficult decisions, some consideration should be given to increasing the grant size of funded projects, even at the expense of not funding some projects at the decision margin.

Finally, it strongly recommended that the COV process for BES be continued on a regular basis.

The Secretary of Energy Advisory Board (SEAB) conducted a study and produced the *Final Report of the Secretary of Energy Advisory Board’s Task Force on the Future of Science Programs at the Department of Energy*, which can be viewed on the Web at http://www.seab.energy.gov/publications/FSPFinalDraft.pdf.

The Secretary of Energy Advisory Board (SEAB) study recommended that the Department of Energy lead our nation effectively through its stewardship and development of critical areas of scientific research and advanced technology by:

- Appointing an Under Secretary for Science;
- Developing and sustaining an increased level of R&D funding;
- Administering its programs using modern management tools and merit-based
- decisions;
- Establishing critically important and inspirational new scientific programs addressing energy production, storage, distribution, or conservation; advanced computation for basic science; and frontier, internationally leading research facilities for fundamental science;
- Improving its congressional, intergovernmental, and public relations and
- communications; and
- Inspiring, attracting, educating, and training the best and brightest as scientists and engineers for careers in DOE-related fields.

Dehmer reviewed the organization of the Department, including the potential new post of Under Secretary in charge of Science, which would be parallel to the Under Secretary over the National Nuclear Security Administration (NNSA). She reviewed the organization of the Office of Science, including the splitting up of the Office of High-Energy and Nuclear Physics into separate offices for High-Energy Physics and Nuclear Physics. And she reviewed to organization of the Office of Basic Energy Sciences, including the creation of the new Scientific User Facilities Division, which will parallel the Material Sciences and Engineering Division and the Chemical Sciences, Geosciences, and Biosciences Division.

Dehmer introduced the new members of the Committee: Sue Clark from the Department of Chemistry of Washington State University, Peter Cummings from the Department of Chemical Engineering of Vanderbilt University, Bruce Gates from of the Department of Chemical

Engineering and Materials Sciences of the University of California at Davis, and Kate Kirby from the Institute for Theoretical Atomic, Molecular, and Optical Physics of Harvard University.

In closing, Dehmer offered the Committee some questions to ponder:

- How will the United States maintain diversity in the federal support of science?
- How will it address large-scale science, including billion-dollar-class facilities?
- What are going to be the hot science topics 20 years from now?
- How will science be done in 20 years, and how will research be disseminated?
- How does DOE improve its brand recognition?
- How will large facilities evolve?

Williams asked how individual labs would tie into BES and how intellectual property should be handled as it crosses from government to industry. Dehmer responded that more collaborative work will be conducted in nanoscience. DOE has engaged its General Counsel in dealing with intellectual property, but the final answers are not yet in hand. Williams noted that Hewlett Packard has been struggling with this question vis a vis academe and would welcome government to the discussion.

Richards asked if the National Institutes of Health (NIH) is trying to poach on DOE biological research areas. Dehmer replied, no. The issue is that NIH's budget is increasing so quickly and that DOE's is remaining flat. DOE's R&D funding is much smaller than that of NIH. If the trend continues, it would make NIH the major science agency in the government, and this situation would raise questions. Stupp noted that territories are getting mixed. Medicine cannot advance without advances in physical sciences. Dehmer went on to say that the issue is that 600 institutions signed a letter asking for an increase in NIH budget. This continued increase will produce a skewing of the funding for science in general.

Plummer commented that the document on DOE stewardship of the labs is excellent and asked how BESAC can help accomplish its recommendations. Dehmer said that BESAC could support the commitment of the Office to accomplish these goals. It requires astute management and policy statements.

Greene stated that, before cuts are recommended, they should be investigated carefully. Dehmer said that, when something gets priority (i.e., cleanup), other things suffer. If an under secretary of science is present at the meetings when such decisions are made, science will get better consideration.

Moskowitz asked what DOE will do to increase the public awareness of the agency and its work. Dehmer said that she did not have the answers to that question. COVs and other actions of this committee will be a part of that solution. Perhaps a specific charge to this Committee will also contribute to this answer.

Hemminger introduced **Harriet Kung** to report on the research needs of the hydrogen economy. She summarized the results of the workshop on Basic Research for Hydrogen Production, Storage, and Use.

At his state-of-the-union address in 2003, President Bush proposed a $1.2 billion research program "so that the first car driven by a child born today could be powered by hydrogen and pollution-free." The drivers for a hydrogen economy are the reduced reliance on fossil fuels and the reduced accumulation of greenhouse gases. At 39%, oil comprises that largest sector of the total U.S. energy supply; transportation is the largest user of petroleum; and domestic production of oil is declining.

The hydrogen economy can be split into production, storage, and use. Today, the country produces 9 million tons per year of hydrogen; the target for production of hydrogen as a transportation fuel in 2005 to 2010 is 40 million tons per year. This production would come from water; solar, wind, and hydro power; nuclear and solar thermochemical cycles; bio- and bioinspired methods; and fossil-fuel reforming. Storage capacities are currently 4.4 MJ/L for gas stored at 10,000 psi and 8.4 MJ/L for liquified hydrogen. The 2010 target is 9.72 MJ/L. Today, the cost of using hydrogen in fuel cells for automotive applications, consumer electronics, and stationary heat or electricity production is $3000/kW; the 2010 target is $35/kW. There are huge gaps in all of these areas.

The hydrogen economy is a compelling vision because it provides abundant, clean, secure, and flexible energy and because its elements have been demonstrated in the laboratory or in prototypes. However, the components do not operate as an integrated network; it is not yet competitive with the fossil-fuel economy in cost, performance, or reliability; and the most optimistic estimates put the hydrogen economy decades away.

A workshop on Basic Research for Hydrogen Production, Storage, and Use was held on May 13-15, 2003. It was charged to identify fundamental research needs and opportunities in hydrogen production, storage, and use, with a focus on new, emerging, and scientifically challenging areas that have the potential to have significant impact in science and technologies. Highlighted areas were to include improved and new materials and processes for hydrogen generation and storage and for future generations of fuel cells for effective energy conversion. The three foci of the workshop were hydrogen production, hydrogen storage and distribution, and fuel cells and novel fuel cell materials. Plenary-session speakers set the stage for the workshop, which had 125 participants from universities, national laboratories, industries, DOE, and other federal agencies.

The workshop goals were to identify

3. Research needs and opportunities to address long term “Grand Challenges” and to overcome “show-stoppers”
4. Prioritized research directions with the greatest promise for impact on reaching long-term goals for hydrogen production, storage, and use
5. Issues cutting across the different research
6. Research needs that bridge basic science and applied technology.

The hydrogen-production panel found that the current status of hydrogen production consisted of steam-reforming of oil and natural gas. CO_2 sequestration would be needed if the targets were to be met this way. Alternative sources and technologies include

- Coal, which is cheap but produces a lower yield of hydrogen with more contaminants (R&D would be needed for process development, gas separations, catalysis, and impurity removal);
- Solar, which is widely distributed and carbon-neutral but low in energy density; photovoltaics coupled with electrolysis is the current standard with an efficiency of 15%; it would require 0.03% of the U.S. land area to serve the nation’s transportation needs;
- Nuclear energy is abundant and carbon-neutral but has a long development cycle.

The panel identified several priority research areas. For the next decade or more, hydrogen will mainly be produced from fossil-fuel feedstocks, so the development of efficient, inexpensive catalysts for fossil-fuel reforming will be key. Modeling and simulation will play a significant role.

The power-conversion efficiency of photoelectrochemistry needs to be increased by reducing losses, and spectral response needs to be extended into the red. Costs need to be reduced in the production of the transparent anode.

Biological systems (plants and microbes) can produce hydrogen from water. What is needed is to learn to make nanostructured catalysts that can mimic biological systems for hydrogen production. Furthermore, nanostructures may allow the high efficiency achieved in thermochemical hydrogen production cycles to occur under less severe environmental conditions in line with the capabilities of nuclear and solar power; the research needs here are to lower the temperature of the reactions and to improve materials.

The hydrogen-storage panel found that the current technology uses tanks for gaseous or liquid hydrogen storage, although some progress has been demonstrated in solid-state storage materials. The target applications are on-board vehicle storage and applications for hydrogen production/delivery. These targets demand compact, lightweight, affordable storage. No current storage system or material meets all the targets. Metal hydrides, such as alanates, allow high hydrogen volume density, but the temperature of hydrogen release also tends to be high. Nanostructured materials may improve the absorption volume, and incorporated catalysts may improve the release temperature. The very small size and very high surface area of carbon nanotubes make them interesting for hydrogen storage. The challenge is to increase the H:C stoichiometry and to strengthen the H-C bonding at 300 K; the issue here is control. Nanoscale materials have high surface areas, novel shapes, with properties much different from their 3D counterparts. They are especially useful for catalysts and catalyst supports. Enhanced hydrogen adsorption on high-surface-area nanostructures may be attained by selective manipulation of surface properties. Nanostructures also have other opportunities for use for hydrogen storage. Theory and modeling can identify trends of behavior, quickly narrow down potential solutions, and thus contribute to the understanding of hydrogen storage. For example, calculations have shown that titanium substitutes for sodium in $NaAlH_4$, a hydrogen adsorbent. The titanium weakens the Al-H ionic bond, thus making it possible to lower the temperature of hydrogen desorption by approximately 100 °C.

The panel on fuel cells and novel fuel-cell materials found that the current status reflects a success in engineering investments. The limits to performance are in the materials, which have not changed much in 15 years. Some of the challenges are the development of membranes that can operate in lower humidity, exhibiting strength and durability with higher ionic conductivity. Cathodes require materials with lower overpotential and resistance to impurities (CO, S, and hydrocarbons) that are cheaper than the current platinum-bearing materials. And reformers also need low-temperature and inexpensive reformer catalysts. Priority research areas in fuel cells include the development of triple-percolation nanoscale networks for ions, electrons, and porosity for gases; electrocatalysts and membranes for oxygen-reduction cathodes that minimize rare-metal usage in cathodes and anodes; higher-temperature proton-conducting membranes with known and acceptable degradation mechanisms; and theory, modeling, and simulation, validated by experiment, for the development of electrochemical materials and processes for solid-oxide fuel cells

Overall, the high-priority research directions identified were:

$ Low-cost and efficient solar energy production of hydrogen
$ Nanoscale catalyst design
$ Biological, biomimetic, and bio-inspired materials and processes
$ Complex hydride materials for hydrogen storage
$ Nanostructured and otherwise novel hydrogen storage materials
$ Low-cost, highly active, durable cathodes for low-temperature fuel cells
$ Membranes and separations processes for hydrogen production and fuel cells
$ Analytical and measurement technologies

- $ Theory, modeling, and simulation

The cross-cutting research directions identified were

- $ Catalysis for hydrocarbon reforming, hydrogen-storage kinetics, and fuel-cell and electrolysis electrochemistry
- $ Membranes and separation
- $ Nanoscale materials and nanostructured assemblies
- $ Characterization and measurement techniques
- $ Theory and modeling
- $ Safety and environment

The workshop found an enormous gap between present state-of-the-art capabilities and the requirements that would allow hydrogen to be competitive with today's energy technologies. Enormous R&D efforts will be required. Simple improvements of today's technologies will not meet requirements. Technical barriers can be overcome only with high-risk, high-payoff basic research. The needed research is highly interdisciplinary, requiring chemistry, materials science, physics, biology, engineering, nanoscience, and computational science. Basic and applied research should couple seamlessly.

This initiative is highly visible, and many agencies are interested and involved. DOE has developed a Hydrogen Program Management Plan that coordinates the efforts of the offices of Energy Efficiency and Renewable Energy, Fossil Energy, Nuclear Energy Research (with its Gen-IV reactor program), and SC. In addition, EERE is issuing a draft Grand Challenge Solicitation on Hydrogen Storage (about $150 million for 5 years). OSTP is considering a Hydrogen R&D Task Force Group to coordinate the activities of the different federal agencies and to develop a taxonomy of research directions to facilitate interagency coordination. The International Partnership for the Hydrogen Economy (IPHE) is holding a ministerial meeting and hydrogen economy dialogue next month to organize, evaluate, and coordinate multinational research, development, and deployment programs. DOE and the European Commission are implementing an agreement on hydrogen research and applications. And the International Energy Agency (IEA) has formed a Hydrogen Coordination Group.

The question is how to get the message out. The report is only half of the job of the Subcommittee. The leaders gave briefings to OMB/OSTP and SC. The report will also support presentations at the American Physical Society, Materials Research Society, and American Chemical Society. *Physics Today* will carry an article by Dresselhaus, Buchanan, and Crabtree, the workshop chairs. The Jim Lehrer Newshour interviewed the chairs. Dresselhaus is currently in Brazil for its annual energy conference. And a Nova television program is planned on the topic.

Hemminger welcomed the report from the workshop.

Kohn said that health is a legitimate concern of the nation, but energy is, also. The emphasis of this initiative is misleading: to make hydrogen-fueled cars. The real job, as this workshop shows, is producing, storing, and employing the hydrogen. He noted that the workshop report had said that 0.3% of the land surface of the United States would be needed, a number characterized as a huge usage. But he did not believe that that area is so great. He went on to note that the nation not only has to replace the 39% of petroleum used for transportation at a time when supplies are dwindling but also has to meet increased demand from a burgeoning population and adoption of technology. This latter concern is especially meaningful in the developing countries. He commented that one does not want the hydrogen too tightly bound in the storage medium and that energy-density theory advancement could contribute to this issue.

Morse asked where EERE is located n DOE. Dehmer replied that it is an office parallel to SC and is under the same under secretary as SC is.

Morse asked what fraction of funding for basic research is expected for hydrogen R&D. Dehmer responded that hydrogen had the least amount of funding (<$10 million) in BES at the beginning of this study. These workshop reports are being used for significant increases in hydrogen R&D. Those increases would be across the entire BES research portfolio (as opposed to setting up a separate hydrogen program). Kung has been the go-to person (contact) for such research support.

Williams commented that Europeans have taken this problem very seriously for many years as have Japan and Korea (which are working on fuel cells) and asked if the United States has plans to leverage off this foreign research. Kung replied that many European and Japanese participants were invited to the workshop. The IPHE will play an important role in such information exchange, and DOE is working on such things as joint solicitations with Japan and other countries.

Moskowitz questioned the word "abundant" as applied to hydrogen. It is abundant as a low-free-energy source, not as a high-free-energy source. Investors do not recognize this difference. It is an energy medium rather than an energy source. Finding the energy source (solar, nuclear, etc.) to use this medium is the challenge. Also, he said, the surface area required comes down to 32 by 32 miles, which is not great, as Walter Kohn pointed out.

Stupp commented that it would be good to have a graph that shows where the United States stands in comparison to Europe and Japan (in industrial investment, for example). Kung agreed that such numbers would show the magnitude of the gap very well.

Bucksbaum returned to the question of surface area needed and noted that the roads that exist for transportation cover a much greater area than what would be required for this initiative. He asked how this report fits into how resources will be allocated. Kung responded that DOE is trying to make this report objective; it is stressing the long-term effects of a hydrogen economy. A strong effort was made to balance research needs and societal benefits. It is hoped that this document will be helpful to program managers. Dehmer said that, when this initiative began, there was no basic research being done in hydrogen. This workshop report is the only document that addresses basic science research in hydrogen production, storage, and use. The initiative will undoubtedly come up with demonstration vehicles but has to go well beyond that; the roadmap to do that will require basic research.

Hemminger brought up a cautionary note about environmental impact: The hydrogen leakage that will occur may affect atmospheric chemistry. He asked if that will be folded into the basic research done. Kung replied that that concern is identified in the report as one that needs more attention. Taylor noted that leakage is a technical challenge; hydrogen is money. There is an economic as well as environmental concern.

Gates commented that it would be helpful to tell the energy costs involved in hydrogen production. Kung replied that it is hoped to improve the discussion of that issue in the final report.

A break was declared at 10:40 a.m. The chairman called the meeting back to order at 11:06 a.m. and introduced **Walter Stevens** to give an update on the Chemical Sciences, Geosciences, and Biosciences Division.

The Division has a budget of $220 million, comprising about 25% of the SC budget. It is divided into three teams: Fundamental Interactions, Molecular Processes and Geosciences, and Energy Biosciences Research, each with a series of focus areas. Stevens reviewed the personnel changes that had occurred during the past year and the distribution of funding among the Division's core activities.

	FY02	FY03 Request	FY04
Chemical Physics	33,285	32,795	33,239
Energy Biosciences	31,190	30,908	31,328
Photochemistry and Radiation Research	26,096	28,605	28,973
Catalysis and Chemical Transformations	24,779	30,870	32,333
Geosciences Research	21,252	20,950	21,232
Separations and Analysis	12,967	14,195	14,387
Atomic, Molecular, and Optical Science	11,815	11,640	12,275
Chemical Energy and Chemical Engineering	10,953	10,795	10,937
Heavy Element Chemistry	7,637	8,510	8,625

The one increase in FY03 is in Catalysis and Chemical Transformations. Theoretical and Computational Chemistry will be added as a cross-cutting activity.

A major activity during the past year was the issuance of the report for the BESAC workshop, Opportunities for Catalysis in the 21st Century, which was held May 14-16, 2002. As a result of this workshop, a solicitation for research in catalysis science was prepared and issued on December 17, 2002. The purpose of this solicitation was to focus on molecular science as it applies to catalysis. It called for multidisciplinary, multi-institutional proposals. It offered $6.5 million to be distributed among universities and national laboratories. The solicitation resulted in 62 multi-investigator proposals being submitted, requesting $49 million for FY03. A multidisciplinary review panel of 28 experts recommended that 11 proposals be funded at the level of $7.5 million for FY03:

- Metal-oxide catalytic functionalities
- Metal-alloy based catalysts
- Molecular-inorganic hybrid material catalysts
- Catalysis informatics
- Inorganic molecular cages: mechanistic principles
- Achieving atomic resolution in nanoclusters
- Understanding the electrochemistry of enzymes
- Energy flow dynamics with femtosecond and nanometer resolution
- Immobilized organometallic interface design
- Hierarchical inorganic structures for site design
- The surface catalysis of chiral synthesis

The results of the solicitation reflects a success rate of 15% on a dollar basis and 18% on a proposal basis. The awards will support 59 PIs in 19 universities and 3 national laboratories, including 42 investigators who are new to the DOE-BES catalysis program. The breakdown of the 3-year allocations is $5.3 million to national laboratories and $14.8 million to universities.

Another BESAC workshop that produced marvelous effects was that on Theory, Modeling, and Simulation in Nanoscience. It resulted in a solicitation for research proposals that was issued February 6, 2003. This was a $6.0 million joint solicitation with the Office of Advance Scientific Computing Research. It resulted in 62 preapplications of which 17 were encouraged to submit applications; an additional 9 were told to submit applications if greater attention was paid to the cross-disciplinary nature of the announcement. In the end, 34 applications were received, representing 280 PIs; some of these applications came from people who had been discouraged. Of the 34, 30 were deemed to be responsive to the call and were reviewed by two panels of 14 reviewers each. Four projects were funded:

- Computational nanophotonics
- Predicting the electronic properties of 3D, million-atom semiconductor nanostructure architectures
- Scalable methods for electronic excitations and optical responses of nanostructures
- integrated multiscale modeling of molecular computing devices

The breakdown of funding recipients is $3.78 million to national laboratories and $1.72 million to universities.

Another important activity was the workshop on Basic Research Needs for the Hydrogen Economy, held May 13-15, 2003.

The COV recommended that BES draw up new BES procedures and guidelines for national laboratory program reviews to produce a more consistent approach between universities and national laboratories in reviewing proposals. These new procedures call for

- Six months before the fiscal year begins, a national laboratory is informed of upcoming reviews for the fiscal year.
- Three months prior to the Review Document due date, the national laboratory is informed of the specific review and is instructed to prepare review documents according to published guidelines. The type of review (mail, panel visit, or both) and due dates are set.
- One month after the Review Document is received, a cover letter and the proposals are sent to the reviewers.
- Three months after the Review Document is received, the reviews from the reviewers are due.
- Four and a half months after the Review Document is received, a debriefing with the division's director and associate director is held.
- Five months after the Review Document is received, a guidance letter is sent to the laboratory with the review summary, reviewers' comments, and action items.
- 30 days after the guidance letter is sent, a response from the laboratory is due.

These merit-review procedures are discussed on the Web at www.sc.doe.gov/bes/peerreview.html.

Kohn asked, from all the solicitations, which of the proposals that were funded involved theoretical studies. Stevens replied that he did not have those specific figures, but about 10% of the Division's investment in university research is in theory and modeling.

Morse noted that some of the budget numbers were for 3 years and asked if the level of ongoing recharge costs is adequate. Stevens responded that none of the projects were funded as high as the proponents requested. **Raul Miranda** stated that the request came to about $90,000 per year per investigator. Morse responded that $90,000 per year is not enough to maintain a strong research activity in any laboratory today.

Williams, asked, given the proposals received, what fraction was fundable. Stevens said, on the order of 40 to 50%.

Flynn asked what the scenario for funding DOE facilities is. Stevens said that BES has a toolkit. Rarely will someone lose a job. Movement to other programs is possible. Often DOE works with laboratory management to guide them toward what is expected and needed. Over years, a decline of funding for particular departments can be a signal. In the past, whole projects have been turned off. Dehmer commented that, in reviews of such facilities, a new director has been installed in 30% of the cases. Stevens noted that the peer review process is another mechanism that is used as well as program management. Often DOE cannot allow such facilities to fail, so changes are instituted rapidly.

Hemminger stated that he did not think that limiting awards to $90,000 per project is reasonable. The COV recommendations were to increase the basic funding level. Stevens replied that the Division has been targeting $135,000 as the basic funding per year. It tries to fund a graduate student, a postdoc, and a summer salary for the principal investigator, which comes to $135,000.

Hemminger asked what the cited “new researchers” were new to. Miranda replied, to the BES core program.

Flynn noted that the piggybacking of experiments is the sine qua non of proposals today except in the case of large projects. Stevens agreed and noted that such piggybacking is watched quite carefully.

Morse said that, if funding were $135,000 per year, overhead knocks it down to $90,000, and fees, benefits, and salaries would leave just $9,000 for instruments, travel, supplies, etc. The case needs to be made to OMB about sole-sourcing such projects and the role of piggybacking has to be explained and accepted.

Hemminger opened the floor to general discussion. Two issues were before the Committee:

1. A COV is to assess the new division within BES. (Volunteers are needed for this COV.)
2. A subcommittee needs to address the second charge (on high-end computation for the sciences). Bill McCurdy and Kate King will be the cochairs.

In regard to the second issue, Stevens noted that a cross-agency panel is also looking at this topic. SC needs the Subcommittee to look at what is going on in computational science and what impacts it will have on BES. How should those developments affect BES budgets, and what should DOE be looking at as it draws up future budgets.

Williams offered the opinion that future increases in computational capabilities will lead to the scaling up of favorite software packages. However, the most important effect will be the ability to do things that could not be done before. An emphasis on this latter capability in this charge letter is satisfying.

Stevens said that what is being talked about is way beyond the theory and modeling workshop. McCurdy noted that several workshops have been held to find the justification for larger computer capabilities. That is not what this Subcommittee should do. It should look at what computation can do to expand the understanding of basic science in such fields in the BES portfolio as nanotechnology and the hydrogen economy. One needs to know what these computers will be used for before calling for larger computers.

Kohn pointed out: (1) Computers and modeling are different. Then there is theory. That is not limited to applied mathematics. Construction of theory is critical. (2) New potentialities can be created by the availability of new computers and software. Those new potentialities can have a tremendous impact on science.

Plummer said that someone is needed on this subcommittee who believes that the advance of science does not depend on the development of teraflop computers. Berrah added that people with a wide variety of perspectives are needed.

Taylor noted that the hydrogen workshop addressed the DOE mission directly. Computing is an important portion of addressing that mission, and this Committee should address the underutilization of computational resources here.

McCurdy noted that Phil Bucksbaum once suggested that theoreticians should have an experimentalist to keep them honest. The presence of experimentalists is very important. Stupp agreed that that is an area that has to be considered carefully.

Moskovitz noted that there is a difference between theory and simulation. Running simulations does not necessarily advance theory. Theory should lead to new science (new physics, chemistry, etc.). Theorists could be left out of the picture here while hours of computer time are devoted to simulation. The most creative individuals should not be marginalized.

Hemminger declared a break for lunch at 12:04 p.m.

Monday, October 20, 2003
Afternoon Session

Hemminger called the meeting back into session at 1:21 p.m. and introduced **John Galayda** to present an update on the Linac Coherent Light Source (LCLS).

The LCLS is designed to produce light pulses of 100 femtoseconds (fs). It will be capable of a spectral coverage of 0.15 to 1.5 nm, going to 0.5 Å in the third harmonic, a peak brightness of 10^{33}, an average brightness of 3 H 10^{22}, producing 1012 photons/pulse, a pulse duration of <230 fs, and a pulse-repetition rate of 120 Hz. An upgrade would allow the production of more bunches per pulse.

The LCLS will use the last kilometer of the Stanford Linear Accelerator Center (SLAC) Linac, producing an electron beam that will go through undulators that produce the X-ray beams for two beam halls. The photon-beam-handling systems will include

$ X-ray transport, optics, and diagnostics
$ Front-end systems (attenuators, shutters, and diagnostics)
$ Optics
$ X-ray endstation systems (hutches and personnel protection)
$ Computer facilities for experiments
$ A laser for pump/probe experiments
$ Detectors matched to LCLS requirements
$ Systems for the first experiments in atomic, molecular, and optical physics

A new configuration has been adopted for the LCLS that adds an additional hall at the end of a new X-ray transport tunnel, leaving room on either side of the main beam line for 8 to 12 additional beam lines.

Since the April 2002 DOE review, the Critical Decision 1 (CD1) was approved in October 2002, the BES 20-year roadmap review was held in February 2003, the SC-81 Lehman/Carney review was conducted in May 2003, and the CD2A was approved in July 2003.

The revised total estimated cost range is $200 million to $240 million, and the revised total project cost range is $245 million to $295 million.

They had good luck in obtaining management personnel. The Chief Engineer is going to be Mark Reichanadter, the Lawrence Livermore National Laboratory (LLNL) LCLS Project Director is going to be Richard M. Bionta, and the LLNL-ANL (Argonne National Laboratory) Project Director is going to be Stephen V. Milton.

The conclusions of the original BESAC reviews were that the LCLS is essential for exploring future science with intense femtosecond coherent X-ray beams. As a result, CD0 and CD1 were approved. The May 2003 review proposed

$ The acquisition of the LCLS injector (including the laser and laser room and the main mechanical systems)

$ Early integration with the SLAC Linac

$ Laser systems assembly and startup in FY05

That review resulted in the long-lead procurements of selected linac systems: the superconducting wiggler, the X-band rf system, and the chicane magnets. It also called for the long-lead procurement of the undulator hardware (including the magnet blocs, magnet poles, strongback, and undulator measurement system), the final “shimming” of magnets at SLAC, and the completion of the delivery of undulators by June 2007. These long-lead procurements (plus spares) cost $30.7 million.

The May 2003 review gave the green light for approval of CD2A in June 2003. This allows DOE-BES to include $30 million in the FY05 budget request. The next DOE review will be held about March 2004; it will consider the formal quantitative risk assessment/management system and settle the baseline (scope, schedule, and cost) for the entire project.

In response to the recommendations of the review committee, planning was initiated to build a second undulator prototype, an undulator vacuum chamber, electron-beam diagnostics, and X-ray diagnostics.

An LCLS Scientific Advisory Committee has been established to guide the FY06-09 funding for construction of experiment stations.

In the LCLS, pulses of electrons in the beam line are subjected to an rf accelerating voltage and a magnetic field in a chicane. This process accelerates the electrons at the back of the bunch more than it does to the electrons in the front. As a result, the bunch is compressed (and shortened) along the line of travel. The current produced by the bunch of electrons increases as its duration decreases. The trick is to compress the successive bunches so that the peak current of each peak is maximized and the length of each pulse is minimized. The eventual hope is to produce a 2- to 3-fs full width at half maximum X-ray pulse with the baseline LCLS design and a simple foil, the number of photons per pulse reduced from 10^{12} to 10^{10}, a pulse length that is adjustable with a stepper motor, precisely spaced double pulses, and a pulse length down to <1 fs.

DOE has asked how the LCLS could be expanded, and a paper has been submitted to the *Journal of Synchrotron Radiation* on future possibilities of the LCLS. That paper postulates an upgraded LCLS to have a spectral coverage from 0.012 nm (5 keV) to 100 nm (0.25 keV), a peak free-electron laser (FEL) power of up to 200 GW, 1 to 60 FEL pulses per electron macropulse, and a minimum pulse duration of <1 fs.

In terms of the SLAC Linac being used as an FEL driver, the LCLS is designed to run at 4.5 to 14.3 GeV at 120 Hz, and the possibilities include

1. 50-GeV beam energy X-ray FEL at 100 keV,
2. Pulse-to-pulse energy variation at 120 Hz, and
3. 300-ns macro pulse with up to 32 micro pulses.

Finally, the SLAC commitment to the LCLS has been summed up by the Director saying that the LCLS could use any SLAC capabilities.

He also described short-bunch generation in the SLAC Linac, noting that the Sub-Picosecond Pulse Source (SPPS) is not an FEL. The rf transverse deflecting cavity has been used to measure bunch lengths. Measured output was 2 H 10^7 photons/pulse; the emittance was 0.4 nm-rad (horizontal) and 0.06 nm-rad (vertical). It proved possible to measure diffraction through an organic crystal with Salol single-pulse exposures. The next SPPS run will go from November 17, 2003, to February 15, 2004.

Berrah asked how often they will have SPPS runs. Galayda replied, about 6 months of each year. The LCLS construction will not require shutdown of the SPPS until January 2006, so it should be running until then. Berrah asked if he had any estimates of its usage in the out years (e.g., number of users and their diversity). He responded, a few hundred users per year. SLAC is calling for letters of intent for single experiments and end stations by next February. The LCLS does not have approval to construct anything yet. The first acquisition might be approved for 2005, so we have to wait for the right time to ask the scientific community for expressions of interest and indications of the experiments they might run.

Richards asked if this project coordinates at all with the proposal of the California Institute of Technology. **Keith Hodgson** answered, no; the Cal Tech proposal is not for an FEL.

Morse asked if the X-ray systems were too hard to reveal protein structures, which is an important capability because it is an essential step to take to get to the next level of understanding of the life sciences. Galayda answered that the X-rays will not be too hard.

Bucksbaum asked what portion of the experimental stations will be funded by DOE. Galayda replied that the LSLS project covers the undulators, the shutters, up-beam X-ray diagnostics, clock lasers, optic properties, prototype detector, inter alia. What is missing is a sample holder, additional X-ray optics, molecular imaging, some amplifiers, etc. Bucksbaum noted that a lot of infrastructure will have to be supplied by the experimentalists. Galayda said, yes. Dehmer commented that, at the time the facilities are baselined, it will not be known what instruments will be needed, called for, or available. This situation is similar to what we are dealing with in the SNS. Hodgson observed that, from the facility point of view, cognizance has to be taken of the President's FY05 budget, but there will be international interest in this project's going forward.

McCurdy said that his understanding was that the pulse would be so intense that some biological samples will be destroyed. Hodgson said that the LCLS will do what is done today with third-generation machines but at higher resolution. With those third-generation machines, you will not have a problem because they deal with millions of molecules. Where you run into problems is where you have just one copy of the molecule (as in the LCLS). The capability to image that molecule has yet to be proven, although simulations indicate that it can be done. It is not the increased resolution that will make the great advances in science over the third-generation machines. What will make the big advance is the very short pulses. If you can make the pulses shorter, the hope is that they will produce detectable scattering before the molecule blows up.

Hemminger introduced **Roy Orbach** to give an overview of the Office of Science. Orbach said the Office was very pleased with the contributions of the Committee. Now the question is what the Office will include in its research portfolio. He asked the Committee to respond to two additional charges:

1. A COV in the new Scientific User Facilities Division of BES, and
2. An assessment of high-end computation.

SC realizes the enormous potential that high-end computing has, referencing a new report (*A Science-Based Case for Large-Scale Computing*, available on the Web at www.pub.gov/scales/docs/volume1_300dpi.pdf). The Committee was provided with the Executive Summary of this report.

He is asking BES to put together a workshop on materials for fission and fusion reactors. The Gen-IV and International Thermonuclear Experimental Reactor (ITER) programs will need materials that can take the huge neutron fluxes produced by these machines. He noted that a new facility at Brookhaven National Laboratory (BNL) is designed to produce radiation shielding (a materials problem) for spacecraft bearing humans to Mars. The question is whether these issues can be addressed by high-end computing through simulation from the chemical-bond to the macroscopic scales. If so, science would not be flying completely blind. The workshop next spring is to determine whether such simulations can be done and what resources they would require. If these materials cannot be simulated, a $100 million to $1 billion facility would be needed to test materials to find the ones with the proper characteristics.

This is not just a question of speed of computation but also of the sociology of science, whether many diverse researchers can work together using a large machine. The hope is that the groups working together would produce findings more efficiently than by parceling out short machine times to individual researchers. Peer review will be used to identify teams of researchers to carry out these simulations.

SC now has a firm date for producing the 20-year roadmap for DOE research facilities, which came out of the efforts of the various advisory committees. That roadmap will give the United States the capability to do research that otherwise would not be able to be carried out. Twenty-eight projects are envisioned; eleven in the first epoch (the near term). CD-0s will be issued for those 11 facilities, and they will be funded on a funds-available basis in the coming years. This decision will be announced by the Secretary of Energy on November 11 at the National Press Club.

The Energy [authorization] Bill is in heated conference between the House and Senate. The effects on SC might be enormous and include high-end computation, Genomes to Life, and other futuristic programs of SC. The compromise bill has to go then to the floors of the House and Senate. An authorization for SC of $5.4 billion is being sought. The House version is $10 million more than the President requested. The Senate version is $40 million more. The difference between the two bills is the need for and support of high-end computation for all federal agencies.

SC has signed a memorandum of understanding with the Department of Defense, which will allow DARPA (Defense Advanced Research Projects Agency) to work with SC to get high-end computer architectures to be available for basic science. This strategy opens up new vendors and leadership-class machines for science applications. The first task will be to determine which architectures will be appropriate for what classes of scientific problems.

Right now, DOE is working on the FY04 budget at the same time as it is submitting its FY05 requests to OMB. Many groups (the American Chemical Society, American Physical Society, etc.) have come forward to explain and defend the importance of basic science. This effort has been quite effective to the benefit to the nation and, indeed, the world.

A healthy relationship exists between SC and the applied-science portions of DOE. The Secretary of Energy Advisory Board (SEAB) looked at how SC works (or should work) with the rest of DOE and issued a report. [See www.seab.energy.gov/news.htm and www.seab.energy.gov/publications/FSPFinalDraft.pdf.] It is an exciting report. Orbach urged the Committee to read the whole report and comment on it, if need be. This report will form a plan for the Department for the next 10 to 20 years. The SEAB committee picked up on the SC facilities plan and recommended that all of DOE have a similar 20-year plan.

Stupp commented that a high-end computing effort by SC that was relevant to the DOE mission would look different from one for the National Aeronautics and Space Administration (NASA). There are some commonalities (e.g., architecture). The directing efforts might not always be in DOE’s favor. Orbach responded that, unfortunately, DOE does not have enough leadership-class machines. DOE tends to be driven by programmatic issues, but all of those issues are areas of basic science. The health of science in the United States is as robust as it is because of its diversity. The National Science Foundation (NSF) is focused on grid computing. DOE focuses on leadership-class machines. Others work with other architectures. The issue is, are we in danger of being focused too narrowly? No. Scientific quality is the basis of competition for time on NERSC. We have set this as a challenge to other agencies, saying to them: Here is what we are doing; now, what are you doing?

Kohn noted that, at the end of World War II, the Navy made a commitment to strong science. That commitment became the model for the NSF. I congratulate you on extending that model. Orbach said that he knew first-hand what Kohn was referring to; his first research contract was from the Office of Naval Research (ONR) 45 years ago.

Williams asked if he would explain more broadly the relationship between mission-oriented and basic science and whether other groups are trying to balance the funding of science. Orbach said that the President’s Science Advisory Committee looks over the budget for balance. They look for overlap but also at the health of individual fields and complementarity. The legislative branch also has committees that exercise oversight. This dual control over the science budget is a blessing that helps ensure balance and efficiency in the funding of science. There is not a formula for striking this balance, but it relies on deliberate consideration and careful explanation. SC does not feel any constraints; it is a healthy environment.

Taylor observed that there is a parallel to what goes on in corporate America. A corporation gets good ideas from exposure to the mission part of the organization, exposing researchers to research opportunities that they otherwise would not be aware of. Orbach responded that there is an exciting synergy there. He has heard from General Electric and General Motors that prototyping (e.g., of jet engines) is too expensive and time consuming. They are hoping that high-end computing will produce cheaper virtual prototypes with much shorter lead times. That type of efficiency is important for the United States to maintain its manufacturing competitiveness.

Hemminger declared a break at 3:10 p.m. He called the meeting back into session at 3:46 p.m. and introduced **Ian Anderson** to present an update on the SNS, a 1.4-MW neutron source that is being built by six national laboratories at Oak Ridge National Laboratory (ORNL).

The SNS will begin operation in 2006. At 1.4 MW, it will be about 8 times as brilliant as ISIS, the world’s currently leading pulsed spallation source. The peak neutron flux will be 20 to 100 times that of ILL (Institute Laue Langevin). The SNS will be the world’s leading facility for neutron scattering. It will be a short drive from the High-Flux Isotope reactor (HFIR), a reactor source with a flux comparable to that of the ILL

All aspects of construction are near or ahead of schedule. The first beam was produced on the drift tube linac at 25 mA, a 1-msec pulse on September 24, 2003. Since then, they have produced a full-energy beam. The klystron gallery has been installed, and three cryomodules have been installed in linac tunnel. The cells are being installed in the ring tunnel. The target room and backscattering beamline hall and tunnel have been constructed. The core vessel was installed October 9; it was finished 22 days ahead of schedule. The inner support structure of the target weighs 24 tons and cost $3 million. It was positioned within 0.006 in., and its height was within 0.002 in. of design specifications.

Sixteen instruments have been approved. Five instruments were funded within the project. Three others (the ARCS, CNCS, and Vulcan) were funded by the instrument development teams (IDTs); the first two were funded by BES, and the VULCAN was funded by the Canadian Funds for Innovation. Five additional instruments (SEQUOIA, SCD, SNAP, NOMAD, and HYSPEC) were funded by DOE/BES. The CD0 for these latter five instruments was approved, and the staff is working on acquisitions for them. For the fundamental physics facility, two instruments have been approved. An additional instrument, a neutron spin echo machine, will be funded by Forschungszentrum Jülich and the Hahn-Meitner Institute in Berlin. Finally, the chemical spectroscopy instrument, VISION, has been approved, and a proposal has been made to the NSF for conceptual design funding.

One instrument is at letter-of-intent stage, the macromolecular crystallography instrument, MANDI. Two new letters of intent have been received, one for the Corelli diffuse scattering instrument with statistical chopping, and the other for a time-of-flight microSANS (small-angle neutron scattering).

In addition, the SERGIS instrument, which uses spin-echo techniques, is under investigation.

Twenty-four beam lines are available. The high-intensity, long-wavelength beams have already been allocated; 16 out of the 24 have been committed. The peer-review process is going to be adjusted to be more stringent to make sure that the user community is behind any proposal made.

Five workshops have been held by the Joint Institute for Neutron Sciences, and three more are scheduled. They covered such topics as

$ Materials Sciences and Engineering
$ Neutrons in Biology
$ Chemistry and Earth Sciences
$ Neutron Scattering for Chemistry and the Chem/Bio Interface
$ Macromolecular Neutron Crystallography

The SNS team is working closely with HFIR and other facilities, covering issues like user policies, access, and critical staff hires. The SNS was also crucial in establishing the Neutron Facility Roundtable, which standardizes access policies and pools resources (e.g., software). The SNS sees its role in such joint meetings as bringing the community together in workshops to work cooperatively on detectors, polarized neutrons (making sure the SNS is polarized enabled), sample environment (what sampling and handling equipment is needed), and data visualization and analysis software.

New, focused projects include an ionization mode gas detector (BNL/ORNL), a lithium-loaded plastic scintillator (Fermi/SNS), and rare earth borate scintillators (Photogenics/SNS).

The staff is trying to make the SNS a full, easy-to-use user facility. To do so, it must provide help to users in data analysis and visualization. It has to look at data and databases because large amounts of data will need to be stored. It has to provide

$ Metadata and data pedigree
$ Data visualization
$ Remote collaboration and remote access so different people in different places can look at the data and analyze them collaboratively
$ Automation and intelligent control of experiments
$ Simulation (in silico experimentation) need to be done across the Grid
$ Distributed computing (Grids)
$ Synergy (bringing together data from different techniques, experiments, and researchers for comparison and combination)

Researchers do not want to look at the raw data as much as a display of the data that readily allows interpretation. A lot of work goes on automatically, turning raw data into interpretable displays. We can make things easy for the casual user by providing this automation and intelligent control. Such visualization of the data makes it possible to get immediate feedback and to make a rapid decision whether or not the experiment was done properly. For this reason, the SNS needs to be put on the Grid, linking data, users, and computational resources. Recently, Thom Dunning put in a proposal to put Oak Ridge on the NSF Teragrid for $3.9 million. NSF asked the proponents to expand the facility to include a hub.

One needs a good source, good instruments, a good sample environment, and good data treatment to get good scientific results. Usually, the source gets good funding, and the instruments get funded adequately. At the SNS there needs to be more of a balance among these components so that good scientific results can be obtained.

A workshop was held to develop requirements to meet users' needs for data analysis, data reduction and manipulation, data storage and management, remote and local access and controls, distributed computing, and Grid and networking services. More than 100 participants attended and represented neutron users, computational scientists, networking experts, other science communities, medical applications, and collaborators from Japan and Europe

Theory, experiment, and simulation need to be put together to get knowledge. The SNS will provide an integrated environment where all the tools and capabilities can be brought together to solve the problem at hand for both expert and casual users. SNS will take the lead but will need support from the community and other facilities to achieve this goal. The SNS will take neutron scattering to the broader scientific community, and it will be a complete user facility.

Morse asked if any of the instruments are bio-directed. Anderson answered, yes, but NIH is not on board for that instrument, although it is being approached for other instruments. Morse asked if it was the National Center for Research Resources at NIH, and Anderson said, yes.

Gates asked about the track record of user friendliness at other neutron facilities. Anderson replied that the biggest headache is data analysis. There is no architecture to do this analysis, and it is often a problem.

Long inquired what type of resources have to be put into the data analysis and how one establishes costs. Anderson replied that priorities will need to be set. One or two people will be needed to start an architecture. Ten other people will be designated to work on data analysis. European and Japanese capabilities will need to be tapped to help solve this problem.

Hemminger stated that, when he started doing synchrotron research, he found that travel to the facility was required to do the experiment and asked why the SNS will be different. Anderson replied that they had been talking about remote interactions with data rather than about gathering data; at least a student would still be required onsite to carry out the experiment.

Cummings asked how he thought automatic and intelligent control of data might occur. Anderson replied that the concept applies to all research done at the source. The researcher does not want the raw data; rather, he or she wants the interpretation or visualization. Cummings offered to provide some ideas on how to do that. Anderson welcomed the offer.

Hemminger opened the floor to public comment. There being none, he adjourned the meeting for the day at 4:36 p.m.

Tuesday, October 21, 2003

Chairman Hemminger called the meeting to order at 8:33 a.m. and introduced **Thom Dunning** to comment on the repot *A Science-Based Case for Large-Scale Simulation* (ScaLeS).

In computers, microprocessor performance is continuing to double every 18 to 24 months, but there is an increasing mismatch with memory subsystem performance and an increasing mismatch with communication subsystem performance. Handhelds are now more powerful than our last generation of supercomputers.

In storage, disk storage capacity is doubling every year, but data-transfer rates are increasing only modestly (a factor of 2 in 10 years).

In the communications fabric that ties together the massively parallel machines, performance is increasing, but there is an increasing mismatch with performance of computational nodes and an increasing mismatch with the needed I/O transfer rates.

This situation represents a mixed blessing. In the scientific applications area, existing computational models are continually being refined, new models are being created, and some of the old models are being rejected. The use of parallelism is increasing. Most codes scale to tens of processors, a few to 1,000 to 2,000 processors, but almost none to 10,000 processors, even though technicians say that this is the only way to build large machines. New mathematical approaches hold great promise, but it takes time to design, build, and verify these techniques.

What are the scientific opportunities? In combustion science, reacting chemical flows constitute a real challenge because of the lack of computational power. Molecular scientists would like to study chemical reactivity and heavy-element chemistry. In materials science, materials design has been a long-time goal that is being closed in on and multiscale materials modeling would allow covering all the scales involved (from the nano to the macro). In nanoscience, it would be desirable to model self-assembly as well as to simulate nanodevices themselves.

The SCaLeS Workshop was held June 23-24, 2003, in Arlington, Virginia. It was organized by David Keyes of Columbia University, and its goal was to assess the major opportunities and challenges facing computational science in areas of strategic importance to the Office of Science. More than 300 scientists and engineers from academia, national laboratories, federal agencies and other institutions participated. Preliminary topical reports compiled from Workshop notes supplied by the topical-group leaders were edited by David Keyes and Phil Colella into a draft report that was iterated with workshop participants plus others. The report is in two volumes:

1. Summary and recommendations, available for download: http://www.pnl.gov/scales/
2. Detailed discussion of scientific opportunities and challenges, available early next year

SciDAC was looked upon as a successful prototype on which to build. Like SciDAC, the workshop participants were trying to connect the scientific needs in SC to hardware infrastructure and software infrastructure in a predictive mode.

The recommendations of the SCaLeS report fall into three groups. The first group constitutes investments in foundations of computational modeling and simulation. It comprised three recommendations:

- Major new investments in computational science are needed in all of the mission areas of SC, so that the United States is the first, or among the first, to capture the new opportunities presented by the continuing advances in computing power.
- Additional investments in hardware facilities and software infrastructure should be accompanied by sustained collateral investments in algorithm research and theoretical development.
- Computational scientists of all types should be proactively recruited with improved reward structures and opportunities as early as possible in the educational process so that the number of trained computational science professionals is sufficient to meet present and future demands.

An example of why these recommendations are important is the fact that, from 1970 to 2000, the ability to predict bond energies increased by a factor of 3 because of advances in theoretical methodology, computational techniques, and computing technology.

The second group constitutes investments in hardware and software infrastructure:

- Multidisciplinary teams, with carefully selected leadership, should be assembled to provide the broad range of expertise needed to address the intellectual challenges associated with translating advances in science, mathematics, and computer science into simulations that can take full advantage of advanced computers.
- Investment in hardware facilities should be accompanied by sustained collateral investment in the software infrastructure for them. The efficient use of expensive computational facilities and the data they produce depends directly upon multiple layers of systems software and scientific software that, together with the hardware, are the engines of scientific discovery.
- Extensive investments should be made in new computational facilities. New facilities should strike a balance between capability computing for those "heroic simulations" that cannot be performed in any other way and capacity computing for "production" simulations that contribute to the steady stream of progress.
- Federal investments in innovative, high-risk computer architectures that are well suited to scientific and engineering simulations is both appropriate and needed to complement commercial research and development. The commercial computing marketplace is no longer effectively driven by the needs of computational science.

New simulation capabilities are typically developed by taking a theory and turning it over to a team of applied mathematicians and computer scientists and comparing the resulting predictions with experimental results, assessing performance, and feeding back any needed improvements. Moreover, the Branscomb pyramid indicates that one needs all sorts of computing power (from personal computers and workstations to frontier computers) to be able to match costs and performance to actual needs, with capability increasing with increasing cost per flop. Virtually all computers made today are Web servers. That technology should be used where it can, but there are some applications where it is not appropriate. This situation is brought about because there are two types of scaling: hard scaling and soft scaling. With hard scaling, one gets a near-linear speedup that is independent of the problem size; in such a situation, one can simply increase the number of processors to deal with the problem faster. Such a case is uncommon. With the more common soft scaling, speed of computation falls off as problem size increases, and the problem size has to be increased to maintain scaling.

The third group covered investments in networking and collaboration technologies:

- Sustained investments must be made in network infrastructure for access and resource sharing as well as in the software needed to support collaboration among distributed teams of scientists, recognizing that the best possible science teams will be widely separated geographically and that researchers will generally not be collocated with facilities and data.

The trend is toward larger, multidisciplinary teams. For that reason, high-speed networks plus Grid and collaboratory software are needed to connect researchers with each other and with computing and data resources. An example of such software is NWChem, a computational chemistry package designed by the Environmental Molecular Sciences Laboratory (EMSL) at the Pacific Northwest National Laboratory (PNNL) to run on high-performance parallel supercomputers as well as on conventional workstation clusters.

He closed by pointing out that, if the United States does not respond to the changes being brought about by the information-technology revolution, someone else will.

Richards noted that Dunning had been talking about computer-architecture personnel rather than programmers. Dunning replied that one also needs computational chemists etc. It is a broad range of skills needed. If one is going to increase funding, some has to go toward human resources.

Long asked whether the computing technologies (the hardware problems) that he referred to are also within the scope of what is being discussed here. Dunning responded that the report was looking at what is done throughout SC. BES should supply individual PCs and workstations. How far up the chain of computer capabilities it wants to go is an open question. The Office of Advanced Scientific Computing Research (ASCR) now provides the high-end computational capabilities.

Moskovitz asked who was taking care of the number-crunching needs of DOE and other agencies. Dunning answered that the politically incorrect answer is the Japanese. They are interested in scientific computing. The federal government needs a more diverse approach to high-end computing. We have gone about as far as we can by linking together web servers.

Williams commented that the whole field of computer architecture is disappearing as fewer and fewer platforms are available. There is no money in inventing new platforms. If one had a fantastic architecture for scientific computing, who would build it? Where would the market come from to sustain the manufacturing investment? Dunning replied that the government would have to step in to fund those costs. It is a serious problem. Something we could do is to work with individuals to tweak their current designs to make them more appropriate for scientific computing (i.e., a dual-use machine).

Plummer asked if he was saying that individuals will not come up with new discoveries; rather that new advances will come from only teams. Dunning responded that individuals will make advances, but they will be supported by teams that build the tools they use to make those advances.

Cumming said that it is important to recognize that short-term gains can be made by sales talks but that the long-term benefit comes from the breakthroughs made possible by advances in computing.

Gates asked how the tool can be made more user friendly. Dunning said that that is not mentioned in Volume 1 of the report, but it is mentioned over and over again in the draft of Volume 2. The technology is there (e.g., Windows^{TM}), but most high-end computing uses a command-line interface. Volume 2 calls for increased investment in user-friendly interfaces.

Hemminger asked if he could comment on investment by software companies. Dunning replied that most of those commercial packages came out of government-sponsored research. The scientific market is not big enough to support the costs of software development and extension. The federal government should make those 20-year maintenance and evolution investments.

McCurdy stated that the real problem is, if we are going to have petaflop computing, it is going to use many, many processors. How we are going to handle this problem is not clear now.

Hemminger introduced **Alan Laub** to describe the SciDAC (Scientific Discovery Through Advanced Computing) program and the High-End Computing Revitalization Task Force .

SciDAC is a $57 million per year pilot program for a "new way of doing science." It is the first federal program to support and enable computational science and engineering (CSE) and terascale computational modeling and simulation as the third pillar of science. (The other two being theory and experiment.) It is the only program that spans the entire Office of Science (ASCR, BES, the Office of Biological and Environmental Research, the Office of Fusion Energy

Sciences, the High-Energy Physics Program, and the Nuclear Physics Program). It involves all DOE labs and many universities. And it builds on 50 years of DOE leadership in computation and mathematical software, such as the development of EISPACK, LINPACK, LAPACK, and ScaLAPACK.

Successful CSE usually requires teams with members and/or expertise from at least mathematics, computer science, and one or more application areas. The language and culture differences on these teams are large; it is hard for a chemist to talk to a biologist. Moreover, the usual reward structures focus on the individual, which hinders the formation and successful operation of teams and makes teams incompatible with traditional academia with its tight departmental structure. The hope is that SciDAC will help break down barriers and lead by example. DOE labs are a critical asset for early success.

SciDAC has been under way for more than 2 years. The first PI meeting was held in January 2002 in Washington, D.C. The theme was to introduce the integrated SciDAC program and to initiate team building. The second annual PI meeting was held March 10-11, 2003, in Napa, Calif. The theme there was to assess SciDAC progress. The SciDAC concept is working; a cultural change is emerging, and new scientific results have been achieved that would not otherwise have been possible.

Some future SciDAC issues are

$ Additional high-end computing and network resources are needed. The initial SciDAC focus is on software, but new hardware is needed now, partly in response to the Japanese Earth Simulator but also to support potential synergistic partnerships leveraging off the success of the SciDAC model (e.g., the ITER decision and the Fusion Simulation Project). In addition, both capability and capacity computing needs are evolving rapidly [e.g., at the National Energy Research Scientific Computing Center (NERSC), which will not be able to keep up with demand much longer].

$ Only limited architectural options are available in the United States. today. Science and engineering needs require architectural diversity. Mathematics and computer-science research will play a key role. Topical or focused computing can be a cost-effective way of providing extra computing resources.

$ The SciDAC program is expanding slowly. Many important SC research areas (e.g., visualization and functional genomics/proteomics) are not yet formally included in SciDAC. Fortunately, a combination of computational nanoscience and materials science is now included as part of the Nanoscale Science Research Centers.

The High-End Computing Revitalization Task Force (HEC RTF) report is still at OSTP. The public version will be issued next month. Industry is wondering what the federal government is going to do. Cray is the only one committed to scientific computing. The overarching goal of HEC RTF is to revitalize U.S. leadership in HEC as a key tool for science and technology. To lead in science, one must lead in computing. The subgoals are:

$ Make HEC easier and more productive to use; it is currently tedious and difficult.

$ Make HEC readily available to those within the federal research community that need it.

$ Sustain the development of diverse new generations of HEC systems.

$ Effectively manage and coordinate federal HEC.

An 80-page plan addresses three subtasks:

- In core technologies, it calls for the development of detailed baseline, moderate, and robust roadmaps for hardware, software, and systems.
- In capability, capacity, and accessibility, it includes the need for "leadership-class"systems that DOE/SC would be a candidate to operate for the benefit of all federal agencies and notes the wide variation in current HEC procurement and operations and maintenance budgets.
- In HEC procurement, it points out some interagency collaboration already (e.g., sharing benchmarks) and suggests the use of total-cost-of-ownership models.

HEC RTF is supporting increased investment in HEC across the federal government and the reprogramming of existing money because of the science that will come out of it.

Richards noted that there is an enormous biological community that is turning to computational approaches. These investments and this team building could offer enormous opportunities to them.

Morse said that biology is following chemistry into this approach. Science collectively is just beginning to map its questions and problems onto these capabilities. One needs to say, "What is the question?" and let the question drive the use of hardware and software.

Williams observed that most computer architects are taking early retirement or retraining as biologists. The only sustainable market for HEC is proteomics. Just to develop a new chip set costs $100 million, even before you gear up your manufacturing and start to crank out products. IBM and HP are aware of the market out there and are pursuing it very aggressively.

Cumming noted that NIH very generously funds individual and small-group computing, but not at the high end. In terms of HEC being applied to biology, DOE is at the forefront because of the Genomes to Life program.

Kohn said that, coming from a scientific culture that deals with many degrees of freedom, he believes that a formulation of the theoretical problem leads you to a computational problem that relates exponentially to the number of degrees of freedom. To increase the number of processes does not buy you anything. Nature does not have that exponential character. The resolution is to get away from this exponential theory, but it comes at a fundamental cost: limited accuracy. This characterization of the natural world has implications for computation. The global lattice gauge theory is an example where you get less accuracy as you increase computing power.

Hemminger called on **Daniel Hitchcock** to describe the planning being done for HEC.

The ASCR Program supports NERSC and ESnet. It develops software for applications and supports facilities, testbeds, and networks. It has conducted a number of workshops and issued many reports to produce a strategic plan. To enable world leadership in science, several strategic issues have to be dealt with:

- Providing high-performance computing and network facilities;
- Maintaining world-class research effort in applied mathematics, computer science, and computer networks (with a 10-year lead time);
- Forging effective partnerships with applications scientists in all of the Offices in SC;
- Developing effective partnerships with other federal agencies;
- Accelerating transition from research to application (10 years is a long time); and
- Providing long-term support of software because the software and the software it is embedded in has to be maintained.

To enable new frontiers in science though simulation, research must be conducted on the mathematics of complex and multiscale systems (e.g., in climate, the type of mathematics that has to be used changes as the grid is refined); on the ultrascalable algorithms for petascale systems; on the computer science to enable advanced computers (a significant challenge); and the computer science to transform petabytes of data into knowledge (disk capacity is doubling each year, but disk I/O speed is increasing very slowly).

As a result of all these challenges, one needs a research portfolio. A spectrum of computer types are needed:

- Experimental computing facilities that provide proof of concept and small-scale research projects.
- Research and evaluation (R&E) prototypes with sufficient scale to enable the evaluation of their scientific potential, to host research projects, and to enable new science for a few brave users.
- High-performance-production capability computers that provide a stable, multiuser capability environment endowed with a large user support, consulting, and training investment and able to provide direct support of the agency mission.
- Leadership-class computers that are a resource for the whole country. Such computers are the most capable systems available for a class of applications, but they support only a small number of projects. They are managed in a manner similar to that for a light source or high-energy physics facility (e.g., with peer review).

IBM has three architectures under investigation and is discussing tweaking several chips to make them more useful for scientific computing. Cray and Sun are also studying special architectures.

One has to look carefully at how long it takes to go from one type of computer to the next. To go from an experimental device to an R&E prototype to a leadership-class machine to a high-performance production capability to a high-performance-capacity machine to a desktop takes about ten years.

Along with this hardware development, one must also provide the needed software. In addition, network-environment research is needed. As an example of this need, consider that it is not clear that the Transmission Control Protocol (TCP) operates properly above 10 GB/s. Research is being performed in end-to-end performance, in high-performance middleware, and with integrated testbeds and networks.

To help accomplish these goals, ASCR has developed a strategy to establish effective partnerships with applications scientists by building on SciDAC; by developing partnerships that are critical to ASCR; by increasing joint program-office collaboration to plan partnerships, such as in SciDAC, Genomes to Life, and the Nanoscience Fusion Simulation Project; and by funding mathematics, computer science, and “glue” that holds collaborative research projects together while program offices fund science. In this strategy, long-term support is a critical issue for the delivery of software resulting from ASCR research as well as application community codes. This support must be coupled to research but is not research.

The software coming out of this strategic effort can be very expensive. It serves a low-volume niche market; one is not going to sell very many copies of a program that runs on 10,000 processors. It has a distributed benefit but a centralized cost. Many previous models have failed. And it is hard to make a case for support services in a research environment.

Long asked him to say more about collaboratories and whether there is any middle ground between jump starting programs like nanoscience and the 10-year development cycle. Hitchcock responded that there will be intermediate usages of the experimental machines and architecture like the Cray X-1, Blue Jean, and the ASCI (Accelerated Strategic Computing Initiative) Purple machine. A lot of work is being done on developing on collaboratories, including electronic notebooks with time-stamped registries. A lot of instruments of the future will include ways to capture data and to move it around, so all the common systems have to work together.

Cummings called attention to community codes that are built up by groups over decades. They represent programming that is too complicated to do on one's own. The development of community codes is a new, important paradigm. Hitchcock replied that, even making a new version of a code that has multiple components is problematic.

Hemminger opened the floor to general discussion.

McCurdy noted that it is BES's theory portfolio that is important. The new charge for an assessment of high-end computation is asking what the right investment in theory is and what SC needs for computational tools. But, he noted, the description of the charge that Orbach provided during his presentation was more open-ended. He asked if he could get a finite scope to the charge. Hemminger said that subcommittees like this one are most successful when they do what they think is best, especially in interpreting the charge. Dehmer said that the Subcommittee had to assess the promise of this new tool. It is known that chemical dynamics can be done faster, but there may be opportunities for new science. The core question is whether this tool can do something that will provide revolutionary capabilities.

McCurdy said that his confusion involved core questions of what long-term investments in theory should be. Hemminger said that he expected the Subcommittee to bring preliminary work to the next couple of meetings and to gain additional guidance as the work progresses.

Hemminger went on to say that the other charge (the COV for the new Scientific User Facilities Division) requires volunteers. Anyone interested in serving on it should make that known.

He opened the floor to public comment. There being none, he adjourned the meeting at 10:49 a.m.

Respectfully submitted, Oct. 31, 2003
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Recording Secretary