Minutes for the
Advanced Scientific Computing Advisory Committee Meeting
May 2-3, 2002, Crowne Plaza Hotel, Washington, D.C.

ASCAC members present:

John W. D. Connolly, Vice Chair
Jill P. Dahlburg
Roscoe C. Giles
Helene E. Kulsrud
William A. Lester, Jr.
Gregory J. McRae (Thursday only)
Juan C. Meza
Karen R. Sollins
Ellen B. Stechel
Warren Washington
Margaret H. Wright, Chair

ASCAC members absent:

Stephen Wolff

Also participating:

Melea Baker, Office of Advanced Scientific Computing Research, USDOE
James Corones, President, Krell Institute
Daniel Hitchcock, Senior technical Advisor, Office of Advanced Scientific Computing Research, USDOE
Janet Kile, Oak Ridge Institute for Science and Education
Michael Knotek, Office of the Under Secretary, USDOE
Arnold Kritz, Physics Department, Lehigh University
C. William McCurdy, Associate Laboratory Director, Lawrence Berkeley National Laboratory
Frederick O'Hara, ASCAC Recording Secretary
Raymond Orbach, Director, Office of Science, USDOE (Thursday only)
C. Edward Oliver, Associate Director, Office of Advanced Scientific Computing Research, USDOE
Walter Polansky, Acting Director, Mathematical, Information, and Computational Sciences Division, Office of Science, USDOE
Jeannie Robinson, Oak Ridge Institute for Science and Education
Rick Stevens, Director, Mathematics and Computer Science Division, Argonne National Laboratory
Linda Twenty, Program Analyst, Office of Advanced Scientific Computing Research, USDOE
Victoria White, Office of High-Energy Nuclear Physics, USDOE

About 40 others were in attendance in the course of the meeting.

Thursday, May 2, 2002

Wright called the meeting to order at 8:37 a.m. She introduced **Raymond Orbach**, the new Director of the Office of Science (SC). Orbach began by stating that large-scale computation is a component of every office in SC. One of the Office's initiatives is to get computation recognized as a central and necessary component of scientific research.

He reviewed the FY03 budget, which is under consideration in Congress. He compared the current budget request with those of other agencies and other years. SC's FY02 appropriation was

$3.288 billion, although that figure included unfunded earmarks, decreasing the available funding. Its FY03 request is $3.293 billion, an increase of $5 million. That works out to (approximately) a zero increase, but it may end up as an increase of 5% because the Spallation Neutron Source (SNS) and other construction activities are on time and under budget; SC hopes to keep those funds for operations. He reviewed the SC FY03 budget request program by program, comparing this year's requests with last year's appropriations and noting an increase of $12 million for the Office of Advanced Scientific Computing Research (ASCR).

The FY03 budget request emphasizes four major initiatives:

- In nanoscience ($133 million, an increase of $48 million), computation will play a major role. There will be five nanotechnology centers. DOE is working closely with the National Science Foundation (NSF). SC can work in sites at the SNS and at other laboratories to look at the nanoscale. The centers will be at Lawrence Berkeley National Laboratory (LBNL), Oak Ridge National Laboratory (ORNL), Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), and Sandia National Laboratories (SNL). Each of these proposed centers is being subjected to a peer-review process; ORNL has completed that process. The money for the SC initiatives is split between the national laboratories and universities. (Of the SC budget, 50% is devoted to user facilities, 25% to research at the national laboratories, and 25% to R&D at universities.)
- For Genomes to Life, $45 million was requested, an increase of $20 million.
- For the new Climate Change Research Initiative, $3 million was requested.
- For Scientific Discovery Through Advanced Computing (SciDAC), $62 million was requested, an increase of $5 million.

The request calls for a strong increase for more operating time and new instrumentation at user facilities ($1.246 billion, an increase of $40 million). This funding will bring the Office to the maximum efficient use of these facilities. It also calls for improvements to the infrastructure ($43 million, an increase of $6 million).

In ASCR, there is a $13 million increase in Mathematical, Information, and Computational Sciences (MICS), supporting the operation of the National Energy Research Scientific Computing Center (NERSC), the advanced computing research testbeds, and the Energy Sciences Network (ESNet). MICS also supports investments in scientific computing research and in high-performance networking, middleware, and collaboratory research.

An essential strength of ASCR is its ability to combine hardware, software, and R&D facilities and staff. SciDAC allows use of tera-scale computing and information technologies across the SC portfolio and includes in its view the physics problems as well as the hardware and software solutions. SC and ASCR are trying to match the computer to the problem addressed, increasing the efficiency of the machine over that of multipurpose machines. The topical computation problem will need a large community effort. As Richard Hamming said, "The purpose of computing is insight, not numbers." The use of the computer has been essential to gaining insight. Computer science brings a great power to all of science. This approach is a switch from solving equations by brute force. Simulations now provide physical insights.

Topical computing is essential for optimization of systems for applications, community-oriented computing, and specifically QCD, where a scientific opportunity exists to combine specialized hardware and software to verify the predictions of the Standard Model for experiments under way at the B-Factory and the Tevitron and planned at the Large Hadron Collider.

SC is at the beginning of putting together its Strategic Plan. The Office covers topics from the very small (the atomic scale) to the very large (the cosmologic scale). This spread was not possible

before. SC began to focus on that *leitmotif* and on computation as a way of gaining power to address that *leitmotif*. SC looks to its advisory committees for guidance on what directions to go in. SC is looking for a 10% increase in its funding each year; that funding has been flat for 10 years. It is also looking at a number of new initiatives, such as nanotechnology, Genomes to Life, and climate change. In Genomes to Life, bioinformatics is the key. The research community is now moving from sequencing to proteomics and will go on to consider the cell as a complete system. This effort will require biology, computer science, and engineering to work together. This advisory committee must help SC determine what architecture issues it should be addressing, and it should assume the attitude that computation is not a service but an inherent part of all the components of SC.

He closed by thanking the Committee for its hard work and service.

Wright had the Committee members introduce themselves to Orbach.

Dahlburg asked if he had any thoughts on the fusion program. Orbach responded that he had given a presentation at the White House the previous day about the International Thermonuclear Experimental Reactor (ITER), the success of which hinges on computational simulations that are impressively similar to the real thing. Simulation assures the success of that program. SC is also looking at dark energy, which offers a number of opportunities. SC used to have a strong educational component (which went from $60 million per year to $4 million). The Department needs to bolster education in science. Half the staff at DOE will need to be replaced in the next 10 years. Something significant was lost with those discontinued education programs.

Kulsrud said that the research community would like to have all those special-purpose computers and asked how SC was going to fund these and influence the manufacturers to pursue that market. Orbach replied that he hoped that Ed Oliver will come with an answer to that. The Department is increasing its budget and establishing centers, but it cannot get the chips built. It is mostly limited to what is commercially available.

White said that researchers in high-energy QCD are working with IBM Research to develop a special-purpose chip (Blue Gene Lite) to apply to high-energy nuclear physics and QCD.

McRae observed that less than 1% of DOE's budget is devoted to advanced scientific computing and asked what he was missing. Orbach replied, nothing; that *is* the problem. The Office is pointing to the different initiatives that would benefit to justify an additional $100 million in funding. Funding initiatives can relieve pressure on the core program and contribute knowledge and capabilities to the core program. McRae asked if he had a sense of what portions of the programs' budgets are devoted to computing. Orbach answered, no. That would be interesting. SciDAC is obviously applied across the system. There is effective coordination across the programs.

McRae asked how technology transfer will work between the secure programs and facilities and the SC programs. Orbach admitted that he was still uncomfortable with that step, which was necessary to ensure security. SC funds a lot of work at the national-security laboratories to keep that technology transfer alive. The Office of Basic Energy Sciences (BES) is closely connected with all of those national-security laboratories. The issue of the vitality of the science done at those labs is essential.

Sollins asked to get back to topical computing and how to avoid making industry inefficient in manufacturing. Orbach responded that, in addition to the philosophical issues you have to deal with to get the maximum knowledge gain, industry also has to make a profit. The people going into industry are coming from the scientific community. There will have to be different architectures, and the funding will have to meet those needs. Where that money should be put to maximize opportunities is what ASCR and ASCAC have to tell us. The Office is expecting to put money into topical centers (the first of which would be for QCD) to provide insights into these questions. The

FY04 budget is now under consideration. The focus must be on the science to produce the best science up front. Then, the Department can make its request and hope that the budget process accommodates the needs.

Giles agreed that the interaction between the centers and the scientific community is important and said that he was pleased to see the discussion of the Strategic Plan. The Basic Energy Sciences Advisory Committee (BESAC) Subcommittee on Performance Measurement recommended that the advisory committees play a role in developing a Strategic Plan. He asked how that will happen; previous organizations did not map well to the expectations of the Office of Management and Budget (OMB). Orbach replied that he was reminded of a quote from Harry Potter: Divination is not an exact science. Congress knows what SC is; the scientific community has done its work well. It is not a top-down organization. It did take a leap forward; topical centers seemed like the best way to go. But the staff of SC wants to know if that is the way to go. OMB is a complex organization. It is to our advantage to make use of their budgetary framework to explain science and its benefits. It is a great challenge to explain what the Department does (and what it wants to do) to the public, to OMB, and to Congress. What can it do that is so special as to warrant public support? Currently, the Department is "sneaking in" to a Strategic Plan. Orbach said that he will be talking with all the advisory committees and asking them to review the plan and to let the Office know if it is going in the right direction.

Meza asked what effects the Earth Simulator announcement has had. Orbach replied that it is increasing travel to Japan. That solicitation was a wake-up call. The Japanese have done a wonderful job of making that machine work. One has to ask if the direction that American computation has taken is the right one and where it should be going. ASCAC might want to sponsor a meeting on that topic: the future of scientific computation. He said that he would support such a workshop.

Lester asked how one decides what the structure would be at a topical center. That decision could be very limiting and could lead to some dead ends. Orbach said that he had no problem with something growing and then dying. The community has to be asked about the best direction. That runs the risk of chasing fads and dead ends. But that is how science works. Various problems should be looked at (chemical bonds, for example) with the hope that there will be some overlap between the needed computational tools and those needed by other problems.

Washington asked if there was an opportunity for DOE to take on a large computational role in global climate change. Orbach responded that the National Center for Atmospheric Research (NCAR) and other players are in the field. DOE needs to consider what it can do best. The climate models are not rigid. He does not know the answers here and would welcome advice.

McRae asked how OMB would look at increasing topical computing versus investment in postdoctoral fellowships and other people-oriented programs. Orbach responded that this was a hypothetical question that he would not like to comment on but acknowledged that personnel are the essential components of any program. The concept of topical computing was latched onto because it addresses a particular area. It is a community approach. But the topical centers are being presented in broad outlines, and the Committee has the opportunity to shape those outlines along the directions it prefers. The program needs to be explained to OMB to engender its support. OMB wants to support the best science. If topical computation is not the best way to go, DOE needs to change direction.

Kulsrud said that she gains a lot from talking with others in the field and in other fields, and she would like to see centers that would bring together a variety of types of people. Orbach said that the dangers of making the topical centers narrow and isolated certainly have to be avoided. The development of new chips by IBM and the issue of scaling are very interesting and could benefit

from the focus of a topical center.

Connolly noted that there could be different types of topical centers, based not only on architecture but also on software. Orbach agreed absolutely and said that he would not separate the two. Connolly noted that the standard molecular dynamics codes are based on the wrong concept and need to be updated. Orbach observed that to do so may require a change in architecture; the hardware and software often go hand in hand.

Sollins commented that the machine in Japan should have increased networking, not travel. The computing community needs more research in networking. Giles added that an important consideration for a topical center would be its accessibility over the network. Orbach agreed, and that is why there is ESNet.

Connolly observed that the International Materials Institutes at NSF are encouraging collaboration, as is done at CERN. Orbach predicted that the nature of international collaboration in the future will be quite different, allowing one to work "at home." He also observed that international collaboration is more than the sum of its parts. There are national ways of doing things. People from different cultures come to problems in different and wonderful ways.

Stechel said that she had been hearing a lot of emphasis on topical centers and efficient computing. What is wanted is more science, not efficiency out of these machines. A paradigm shift is needed, with simulation integrated into the experimental process. Should these centers drive this paradigm shift or more efficient computing? Orbach responded, both. The increase in efficiency was to provide more insights and understanding into the problem areas. ASCAC needs to tell us how to go about it.

Wright asked if he wanted ASCAC to make a formal response to him about this issue. Orbach said that he wanted ASCAC and Oliver to work this out. That is where the leadership lies.

Wright loosely quoted Donald Knuth, "Premature optimization is the biggest source of programming inefficiency," and suggested getting away from the terminology of "topical" and taking a more general approach to the problem. Orbach responded that that was an excellent suggestion.

Dahlburg observed that a previous report of this Committee suggested that different algorithms might be the best way to organize the centers. Orbach replied that this is the type of suggestion we need.

Wright commented that the Committee has an important role in defining the role of computation and mathematics in science and has been effective in that role. A break was declared at 10:26 a.m.

The meeting was called back into session at 11:00 a.m. with the introduction of **Edward Oliver**, Associate Director of Advanced Scientific Computing Research. ASCR will try to grow the core program, although the President's budget is initiative-driven. Support for the core program has declined 50% during the past years. The Office will develop partnerships with other offices in SC and also enhance coordination with other agencies. It seeks to achieve excellence and innovation in everything it does, exhibit consistently high standards to all existing and prospective research performers, and fund the best research and principal investigators regardless of affiliation.

In FY01, ASCR initiated the software-infrastructure portion of SciDAC with $61 million, initiated computational biology research efforts in the Microbial Cell Program, upgraded NERSC to 5 teraflops, and acquired the IBM Power 4 hardware (located at ORNL) for evaluation and scaling studies. In FY02, the ASCR budget went down $7 million; nonetheless, ASCR issued a research call for early-career principal investigators, conducted six Genomes to Life workshops with the Office of Biological and Environmental Research (OBER), conducted the Mission Computing Conference [discussing with the Department of Defense (DOD), the National Aeronautics and Space

Administration (NASA), and the Accelerated Strategic Computing Initiative (ASCI) the barriers to high-end computing], organized joint workshops with BES and the Office of Fusion Energy Sciences (FES), approved the LBNL proposal to manage and operate NERSC for the next 5 years, and convened the first SciDAC principal investigator meeting. In FY03, it hopes to launch the Genomes to Life computational component in partnership with OBER (requesting an additional $12-13 million for the year); initiate a computational nanoscience partnership with BES (as part of SciDAC); provide topical, high-performance computing resources (as part of SciDAC); and develop and propose an SC strategy for high-performance networks.

The early-career principal investigator program elicited a lot of interest: 132 grant applications were submitted (probably ten times what can be funded), with 63 in applied mathematics, 47 in computer science, and 22 in network research. Peer reviews will be completed June 20, decisions will be made by July 1, and research efforts are to start September 1.

ASCR has funded an HBCU [Historically Black Colleges and Universities] initiative for a long time with the goal of increasing HBCU participation in ASCR research. Visits are being made to a number of HBCUs, and outreach is being coordinated with the Office of Science Education.

The MICS budget request asks for $58.4 million for facilities (an increase of $1.3 million), $52.7 million for base research, $8.6 million for computational biology (an increase of $5.6 million), and $42.7 for SciDAC (an increase of $5.3 million).

Topical computing centers were cited as "a big thing." They are envisioned to provide effective and efficient computing resources optimized for a set of scientific applications, focal points for scientific research communities, and a key element in the SciDAC strategy. The Office's strategic research partnerships are expected to bring terascale simulation to bear on all major science issues facing SC. The Office expects to develop and implement its strategy for high-performance computing and networking. It also wants to grow the base research activities at the levels needed to meet enhanced expectations.

The staff situation is significantly improved with the addition of Gary Johnson to manage the Advanced Computing Research Testbeds (ACRTs) and computational biology, and John van Rosendale to manage visualization and data management. The Office still has two vacancies to fill, the Director of MICS and a manager of the Applied Mathematics Program.

Washington asked how specific advisory subcommittees should be in specifying funding levels. Orbach said that they should be fairly specific but flexible. Managers need to know if a $10 million or $100 million program is being suggested.

Washington noted that NSF is starting to probe the future of architecture and asked if DOE talks with them. Orbach replied affirmatively. DOE representatives meet with them on a regular basis, and DOE belongs to several interagency groups.

Giles called attention to the distinction between base program and initiatives and said that it is important to explain the value of the base program. Orbach replied that he thought the new administration is willing to listen. Sollins observed that it is difficult to get increases in base-program funding even for NSF. The common strategy is to do initiatives and to roll them into the base program 4 to 5 years down the road. McRae asked why it is so difficult to increase the base-program funding. Orbach answered that it is because base-program funding sounds like business as usual; it does not sound different and new. Connolly agreed: the weakest argument that can be used is that more of the same is going to be done.

Kulsrud asked how DOE is going to make topical computing sound new and acceptable when it was refused funding before. Orbach noted that it was not rejected explicitly. No one made a specific rejection of the concept, but DOE did not get the money for some other reason. The timing was not

right.

Stechel suggested that the relevant question might be, "What is really lost when you do not expand the core program?" Orbach replied that those arguments have been made. The link can be made to, say, the decline in PhDs. The problem is that many such links are nebulous.

Meza asked if anyone in ASCR is tasked to forge the strategic partnerships. Polansky responded that the Office follows a business model for networking that has been in place for 15 years. It may need to be updated. A DOE-wide workshop is being conducted to investigate that issue.

Wright noted that ASCAC's prior reaction to topical computing was skeptical to negative and asked why this idea has come back again. Orbach responded that some facilities are needed and science research programs need to be grown and their support expanded. Ideas that were considered were a mathematics flagship center, enlarging the current flagship facility, and making NERSC more available to the material science and QCD community. DOE needed something to support, and it happened to be called topical computing. Wright said that there is great concern that topical centers will be short term and a waste of money. Orbach agreed that it is not a smart move to give the QCD community a machine with a lot of memory that they do not need. Wright went on to say that people use the same algorithms over and over. There are other ways to carry out these solutions. Sollins noted that, if you are in a special topic community, you can be saddled with a computer that cannot do some of the things you have to do. Dahlburg expanded: There exists a portfolio of facilities. The question is how to expand that portfolio to meet all needs.

Stechel asked what caution flags would be seen if it were known what these centers are going to do and what they are going to be capable of doing. Orbach responded that, in the aerospace world, a special-purpose computer is provided, and the work is done in a timely fashion. Stechel commented that it seems as though the cart is being put before the horse; one needs to know the computational needs before setting up these centers. Orbach countered that the Department is not going to buy something that is not needed. Wright noted that it is the Committee's duty to question this decision. Some people ask for something before they fully know what they need.

Connolly said that new approaches are needed, and that a topical center could include such approaches. If one has the right people and good coordination, one can end up with something very useful.

Giles noted that different perspectives are engendered in a community depending on whether a machine is perceived as being "owned" by that community or it is remote and shared. A danger exists that a computer community will see the way to get the computer facilities that it needs and that those facilities would then not be made available to anyone outside the community.

On the other hand, Dahlburg observed, a computer or topical center can be thought of as a tool for doing research, an experimental platform. Then the "mine" aspect goes away.

Meza cautioned that the first thing the Committee heard about last year was "special-purpose computers." If this concept was broached in terms of a balanced system, it would be a different story. He stated that too many of these topical centers have algorithms that they have a commitment to and an investment in and they are unwilling to make any changes in the standard way of doing things.

Wright introduced **Jill Dahlburg** to present the report of the Facilities Subcommittee, which has been assessing the quality and roles of ASCR facilities like NERSC, ESNet, Chiba City, and the ORNL Center for Computational Sciences. A report was prepared by the Subcommittee summarizing the results and findings of its questionnaire and workshop. The main finding of the Subcommittee is that each of the four facilities evaluated is among the best in the world in its respective category. The Subcommittee found that the ASCR facilities and the related spin-off

research efforts contribute to the missions of DOE in an outstanding manner, and they profoundly and positively affect high-performance computing activities (e.g., fusion research and the Grid) worldwide. The Subcommittee recommended that:

1. ASCR should retain focused commitment to high-end computing in the service of DOE SC missions.
2. ASCR should build on its present plan to develop a Strategic Plan for the next-generation, high-end, 21st-Century, multi-user, mission-driven computing environment.
3. ASCR should develop an integrated allocation strategy for its computational resources. This allocation process should seek to ensure that each machine is filled to the greatest extent practicable with high-priority SC jobs that are not feasibly run on smaller machines.
4. SC researchers should be encouraged by ASCR to procure both midrange and low-end machines/clusters with individual-program funds.
5. ASCR should embrace a cohesive networking and resource-allocation approach for computing infrastructure as a way to provide the most uniform interface to all the types of computing facilities that are encompassed by ASCR. To this end, ASCR should continue to incorporate advances in networking and resources integration as they develop and should encourage enhanced research efforts in new architectures and networking capabilities.

On April 19, the Japanese government announced the installation of the Earth Simulator that, according to a *New York Times* article, "matches the raw processing power of the 20 fastest American computers and far outstrips the previous leader." In light of this new development, the Subcommittee decided to (1) consider its report an interim one; (2) re-address the future roles of ASCR facilities by considering their application to nanotechnology, computational biology, fusion, climate modeling, and QCD; (3) initiate in-depth discussions with vendors; and (4) report its findings to the Committee at a later date.

Wright asked the Subcommittee to update its report by the end of May.

Washington suggested that the Committee should give advice about funding levels, not just saying that there should be more of this and that. Dahlburg agreed and asked him to contribute such figures to the report.

Washington noted that the United States has a month of time on the Earth Simulator during the next 5 years. The U.S. climate research community has been changing all of its codes to parallel architecture and does not want to reverse that course. The Japanese government has agreed to change the coding back for a vector computer. The Earth Simulator will not be an easy computer to use. It has no mass storage and no telecommunications. It represents as narrow a topical center as you can get. The operators have a strict requirement to provide a new set of simulations for the next IPCC [Intergovernmental Panel on Climate Change] assessment, getting down to a very fine resolution. He hoped that this new facility in Japan was a wake-up call to the United States. The Japanese government has made a big investment in this facility. The U.S. facilities need to be upgraded.

Lester commented that it would be good to re-examine how the U.S. decision-making led to where the country finds itself today. Dahlburg reflected on the Texas Instrument machine that died when Cray came along with a faster machine with more memory and noted that the United States went down an excellent path for good reasons.

Wright stated that the Committee needed to vote on the interim report of the Facilities Subcommittee. Lester moved, and Meza seconded, to accept the interim report. The motion passed unanimously.

Wright opened the discussion to the public. Arnold Kritz commented that it would be good to

know what fraction of the scientists are using NERSC and Oak Ridge and what fraction are using local (topical) computers and stated that the offices of DOE should be asked to pay for the topical computers.

Stevens said that he was perplexed by the day's discussion. DOE has not been a big supporter of computer architecture. DOE needs to embrace architecture as a fundamental part of the core program. That can be done. NSF excluded architecture research; there is a hole. The NSF Cyberinfrastructure Blue Ribbon Panel is likely to recommend up to eight high-end computing centers. The DOE centers will have to differentiate themselves from those NSF centers. How to do this is an important question.

McCurdy said that the discussion of topical computing is appropriate. The main question is how to grow computer capacity in SC. There is a political dynamic involved. Another assumption is that architectures map onto disciplines, but that is not the case, say, in chemistry. Architecture maps onto algorithms, not disciplines. The appearance of the Earth Simulator is important; DOD and others are holding meetings to determine how to respond.

Connolly noted that the Environmental Molecular Sciences Laboratory is already operating a topical center. It chose its hardware to optimally run the software they wanted to run. That seems like a reasonable model.

McRae stated that topical computing is a second-order problem. The first-order problem is increasing the budget for advanced computing.

Sollins observed that there are supercomputing centers, topical centers, and workstations. The vast majority of runs that used to be made on supercomputers are now done on workstations. She asked the Committee to think about how those tools are paid for and emphasized that there are many categories of computers to be funded.

Wright said she worried about the people needed to do all the things being proposed. Education in science needs investment. Education, training, and people constitute a vital question. Stechel stated that, at a recent panel meeting, the major recommendation was that the U.S. has to develop the people.

Wright declared a break at 12:30 p.m. and called the meeting back into session at 2:02 p.m. She introduced **Juan Meza** to report on the Biotechnology Subcommittee. He turned the floor over to **Mike Knotek** to report on the Genomes to Life program roadmap. The biologists are just taking their first steps into the area of computational science and do not yet understand fully the promise and capabilities of the technology and, therefore, their needs. The advent of the genomic revolution has changed science profoundly. One can never look at a problem of biological understanding in just the same way again. Indeed, sequencing has been turned into a commodity.

A large range of investments has been made in genomic technology:

- Capillary electrophoresis technology used to sequence the genome,
- Large insert cloning technology,
- cDNA library sequencing,
- Microbial genome project, and
- the Joint Genome Institute's contributions to genome sequencing.

The first phase is now ending, and genomic information is readily available. The next, transforming phase is beginning: the understanding of full, complex biological systems. The cost is down to 1 cent per base. The agricultural community now wants to sequence every genus of agricultural interest. This new biology will require large computers and many disciplines to go from the genome to the proteome to the cell and to organism and microbial communities. The other part of this effort is the regulatory network; 95% of the human genome is not coded; that is where the

regulatory system operates. The system-regulatory processes need to be understood.

Biology has changed into an information-rich science that will have high data densities (needed to interrogate complex systems), high-throughput technologies (essential to current biological research), and new research instrumentation and methods [which are rapidly emerging (e.g., protein and nucleic acid arrays, proteomic methods, and high-resolution and high-information imaging)].

Examples of what biologists think is important and interesting today include the precise structures that are encoded in the genomes of microbial cells, many of which are at the nano scale; biology will look at the genomic instructions and study how those instructions determine structure and function. Genomic/proteomic analyses can elucidate new mechanisms, and mechanisms can enable engineering (precise, automatic control at the submicron level). The primary goal of the Genomes to Life Program will be to determine how the genetic program controls the nanostructures, and how people can engineer it.

Only 40 genes are involved in the early phases of the development of the sea urchin embryo. Genetic networks and their regulatory sequences control cell determination, interaction, and function. Through experimentation, one can build a complex predictive model with many "circuits," each of which is a system regulator on the genome. At a critical point in development, one of these circuits kicks in and triggers a series of actions that take the organism to the next step of development, at which point thousands of genes might operate.

Such a model, complex as it is, still leaves much to the imagination, but it is as far as one can go using human intuition. What will be needed are perhaps dozens of facilities, both large and small, tied together with a computer network so they can carry out such tasks as the analysis of multiprotein complexes, mapping and modeling gene regulatory networks, combinatorial chemistry, molecular imaging, production proteomics, and large-scale protein production. These tasks will require protein production, a high-throughput proteomics facility, and intermediate-scale imaging facilities.

The roadmap for going forward has resulted from a series of workshops. Systems-biology research will be made up of experimental and computational hierarchies that will become increasingly codependent as the research community models greater biological complexity. The work will break down into three computing domains:

1. Bioinformatics, a data-intensive application;
2. Biophysics, an extension of the protein-folding world which is compute-intensive; and
3. Biosystems, which involves complex-systems modeling.

The Genomes to Life program seeks to understand protein machines, regulation networks, and the microbial community through these three domains, but faces a number of challenges. In bioinformatics, researchers will encounter vast, heterogeneous data sets and legacy systems that do not interoperate or scale. The whole data-management system will have to be redone. In biophysics, researchers already need more computation, better algorithms, and new theory. In biosystems, there will be too much data not to have models. This situation will require a difficult culture change for biologists, who are accustomed to experimentation. They will be dealing with a short parts list (about 1500 entities), but complex systems will be produced by very complex combinations of those parts.

The biology problem space goes from first-principles molecular dynamics to evolutionary processes. Computing is the only way to deal with such a complex problem. The computational infrastructure will include community databases, tool repositories, community users, special-purpose computers, and general-purpose computers, all attached to a terabit network.

He summarized his presentation by pointing out that:

- The science has changed.
- New capabilities and resources are needed.
- Its history and current thrusts position DOE to make major contributions.
- Genomes to Life provides the rationale and nucleus of a broader program.
- Biological and Environmental Research Advisory Committee (BERAC) and ASCAC should move to recommend specific action on a bold new program incorporating new facilities and resources.

Implementation and management of the program will require planning and involvement by BERAC, ASCAC, and the broad scientific community using an open, peer-reviewed competitive process and the strong integration of sites, laboratories, and users across disciplines and across the current boundaries among national laboratories, universities, and industry. New approaches will need to be tried.

Wright asked what the request for FY04 was. Knotek answered, $36 million and $5 million in ASCR. Wright asked how much of that was for the national laboratories and how much for universities. Knotek responded that the selection process will be competitive.

Washington commented that the biology part is a very high priority of BESAC. The computational aspects are going to be enormous.

McRae asked what is going on at NSF, at the National Institutes of Health (NIH), and in industry. Knotek replied that industry is into proteomics in a huge way. NIH is interested in protein structure to lead to drug therapies. DOE is going after microbes, especially those that have energy applications. John Houghton (DOE Office of Science, Genomes to Life program) expanded on the theme: coordination and planning meetings and workshops are held for the involved communities. Knotek added that there is an enormous investment, but there is no strategic document, as we have for Genomes to Life. Houghton noted that DOE's strategy was worked out in close cooperation with the other agencies. There is nothing in the Genomes to Life plan, for example, about protein folding.

Juan Meza then discussed the Biotechnology Subcommittee's assessment of the roadmap. The roadmap is in a draft version now; it is a well-organized report, broken down into three major areas (bioinformatics, biophysics, and biosystems). The larger vision is still not well-defined, however. The roadmap still needs to develop a strong set of drivers and to define and/or quantify the Genomes to Life goals more clearly.

The bioinformatics section offers the greatest level of detail because it is the most mature area. It was not clear what the data requirements were or whether this was a limiting factor. Furthermore, it was not clear what new capabilities were needed or what the current limitations were.

The biophysics section offers the best argument for computational needs. Molecular dynamics and quantum chemistry are obvious needs but there are likely other areas, also. It would be useful to quantify the computational needs for these areas. Also, one must ask whether anyone has looked at the need for numerical and algorithmic advances.

The biosystems section is the least mature field. Here, it was not clear what the connections between the various sections were. The goals still need to be set and clarified, and the relationship with current systems-biology efforts needs to be established.

A good management plan is included, of which outreach, education, and training are likely to be important components. It would be useful to have a stronger argument for computer resource needs; networking requirements are not given; and storage requirements are not justified in the text.

The recommendations of the Biotechnology Subcommittee are:

- Develop a clear set of drivers that help to explain the Genomes to Life goals;
- Quantify the Genomes to Life goals and requirements, where possible;

- Develop a list of computer science and mathematics challenges or barriers to achieving the goals;
- Define the relationship between the research goals and the Genomes to Life goals;
- Develop a plan for interconnecting the first three goals; and
- Hold a meeting to discuss higher-level strategic issues.

Wright asked how much science had been done on this in the past year. Houghton responded that two solicitations had been issued last year and a new, big solicitation is on the street now with $15 million for the national laboratories and $15 million for others. A number of research projects are ongoing now. Knotek added that five microbial systems are being studied to see what proteins are in play and what they do. The Microbial Cell Program (the Genomes to Life precursor) made great progress looking at processes that occur within a cell.

Wright asked what kind of advice would be sought from ASCAC. Knotek responded that this field is really new to most biologists. They now have the whole genome. Soon they will have information on the whole cell. They will need visualization, data management, etc. to perform biology. They will need to learn how to use computational tools. ASCAC has to work with them constantly and needs to contribute computing people to their working groups.

Stechel noted that there will be a lot of impacts on other disciplines and asked if anyone is looking at how the new capabilities can be shared with other disciplines. Knotek said that the obvious beneficiary is nanoscience. A big push will be made to link arms with the nanoscience community. However, it is not very mature; the human genome has only been known for a year, and only 50 to 100 microbes have been done in that time. This is very new stuff. The biological community has gone through a time warp and is trying to figure out where it is. In 10 years, computer scientists will *be* some of the biologists.

Kulsrud commented that the Society for Industrial and Applied Mathematics (SIAM) recently held a meeting on data mining; applied mathematicians are aware of these issues. Stechel asked if there was a possibility of developing someone who was not only a computational biologist but also had the computational skills to understand computational material science. Knotek said that there are definitely some crosscutting skills. Computer scientists have to learn domain science to understand how their tools fit. The dialogue is premature at this time. The field is in the "can be" state; it will mature into the "should be" state and then on to the "will be" state. Meza noted that education and training (e.g., through postdoctoral fellowships) will be major components of that maturation.

McRae asked why DOE should be involved in this area. Houghton responded that, sometime this century, our civilization will see a zero-net CO_2 energy system. Advanced biological techniques will help bring about that system *and* will reduce legacy wastes. Several DOE missions will be affected and advanced by this science and technology. Wright called attention to the fact that the DOE Computational Science Graduate Fellowship Program has seen a big shift toward computational biology in recent years.

Wright called upon **Gregory McRae** to report on the SC-Wide Issues Subcommittee. He asked for (1) volunteers for the Subcommittee and its working groups and (2) issues that should be addressed.

Wright asked Oliver if anything had been changed in the charge to the SC-Wide Issues Subcommittee with the ascension of Orbach. McRae responded that he had asked Orbach that question and that Orbach had left the response open-ended, saying that he would welcome any advice.

Wright called upon **Jill Dahlburg** to report on the Subcommittee on Integrated Simulation for Fusion Modeling, a joint ASCAC/FESAC [Fusion Energy Sciences Advisory Committee] effort.

About 15 people are on the Subcommittee. Its first meeting is scheduled for May 23, and another meeting is planned. The first meeting will address what needs to be integrated in the fusion community. Orbach had briefed the White House on ITER the day before this ASCAC meeting. Tremendous amounts of knowledge are expected from operating this machine. It will take 10 years to build and will last for 20 years. Simulation will play an important role in its use. In fusion now, a number of physics regions can be modeled (edge, confinement, etc.). A lot of simulations have been made of each of these regions. What is needed is the integration of the models of these regions.

Lester asked what progress had been made over time. Dahlburg responded that, during the past year to year and a half, an understanding of the Tokamak plasma has been achieved. With ITER, a long-enough containment and high-enough heating will be achieved to produce fusion.

Wright introduced **Ellen Stechel** to talk about the upcoming joint ASCAC/BESAC workshop on theory and modeling in nanoscience. BESAC and ASCAC are conducting a workshop on advancing the frontiers of nanoscience through theory, modeling, and simulation. The objectives are to identify new scientific opportunities, the case for growth, and the needed resources, as well as to establish a substantive and intellectual relationship among computer science, the mathematical sciences, and nanoscience.

In February 2002, the decision was made to hold the workshop. In March and April, the workshop was planned and participants were invited. It will be held in May, and the workshop report will be published in June. In August, a major workshop will be held involving the nanoscience and applied mathematics/computer science communities. This workshop is a move to define what will go into the FY04 budget request. In November, a joint funding opportunity in computational nanoscience will be announced ($3.0 million from ASCR and at least a similar amount from BES). The first awards in computational nanoscience will be made in April 2003.

Each of the national laboratories was asked to respond to a questionnaire that asked:

- Why would it be good to invest now in theory and modeling in nanoscience?
- What are the most important intellectual challenges and opportunities in theoretical and modeling in nanoscience necessary to advance the field?
- What would be the plausible impact of an expanded program at DOE in theoretical and modeling in nanoscience? What scientific dividends might be gained by the investment, and what science might be lost without the investment?
- What are recommended thrust areas for a new DOE program in theory and modeling in nanoscience?
- Given the considerable intellectual challenges, why should one expect such a program to successfully have impact on the field of nanoscience? What might that success look like? What are some critical success factors? (How are we going to know we have succeeded?)
- Among the recent research in theory and modeling in nanoscience or closely related applied mathematics and computer science, which papers do you consider to be of greatest significance and why?

Stechel reviewed the schedule, structure, and methods of the workshop and the demographics of the participants. A number of excellent mathematicians are being brought in. The workshop will have invited speakers on a range of mathematical topics; a panel discussion of the role of mathematics and computer science in the nanoscience initiative; and breakout sessions on

- Well characterized nano building blocks;
- Complex nanostructures and interfaces;
- Dynamics, assembly, and growth of nanostructures;
- Crossing time and length scales;

- Fast algorithms for electronic structure and long-range forces; and
- Optimization and predictability.

Connolly asked if this information was on the Web. William McCurdy, co-chair of the workshop, responded that it was not but could be e-mailed to anyone who desired it.

Wright asked about a similar workshop held by NSF two years ago. McCurdy responded that the upcoming meeting focuses on theory and modeling, which are essential for understanding and exploiting nanoscience. The workshop will add considerably to the BES portfolio. Stechel added that the workshop is an opportunity for computer scientists to bring issues to the table rather than waiting to be told what issues are to be addressed. McCurdy went on that the workshop will determine the overall scope of nanoscience as well as the theory and modeling inroads that could be made. It is an attempt to introduce computational and applied mathematics to the investigation of the nanoscale. It will forge a real intellectual relationship between the two offices (BES and ASCR).

McRae noticed that the workshop made no mention of large databases. Stechel responded that those types of things will fall out automatically; the greater challenge will be defining the problem from both the computational and scientific sides. McRae asked how this differs from what is already going on at Materials Design in Canada. Stechel said that the topic at hand is not computational materials. The purpose here is to understand how one goes from the small scale to new functionalities and properties. McCurdy noted that the charge to some of the speakers was to bring out the needs of advancing capabilities such as grasping nanotubes. The speakers are aware of the commercial efforts and will go on from there.

Stechel noted that a recent international survey on molecular and nanoscience modeling showed that the field is not as mature as some would have us believe. The whole task of the workshop is to outline what is new. McRae said that there should be someone like John Rogers to speak on databases.

A break was declared at 3:55 p.m. The Committee reconvened at 4:30 p.m. **Warren Washington** spoke on the Digital Gift to the Nation, a concept put forward by Lawrence Grossman (former president of the Public Broadcasting System) and Newton Minow (former chairman of the Federal Communications Commission) in a report with the same title. Those authors made an analogy between the Morrow Act (which funded the land-grant colleges out of revenues from the sale of federal lands) and the funding of new learning techniques and education in the arts and sciences from revenues from the sale or lease of the radio spectrum. The concept has been endorsed by many university and government leaders. The National Science Board (NSB) has received a request from Congress for a recommendation by June 1 on this proposal. All federal agencies will be asked for comment. An educational component from DOE might be possible. Several issues have been raised: Should the Digital Opportunity Investment Trust be located in the NSF or elsewhere? Everyone agrees that this is a good idea, he said. The NSB panel that is considering it will probably not come down on one side or the other. The NSB will review and approve a draft report and send it on to Congress.

Sollins asked how the spectrum should be sold in light of the disaster that the European sale several years ago turned out to be. She noted that serious economic questions are involved. Washington replied that the mandate of the NSB panel is only on how to use the money.

Giles asked who the "giver" of this gift was. Washington replied that the term came from the title of the report.

Wright asked him what he would like from ASCAC. Washington pointed out that the report spells out a large number of ways that the money could be spent. He believed that the NSB panel should recommend a general mandate, and it would appreciate comments from people and groups

like ASCAC.

Sollins asked if the sale was to be a one-shot deal with the proceeds going into a trust fund that eventually might run low, resulting in requests for public funding 10 years down the road. Washington said that he did not believe that this was yet clear. Sollins asked about the length of the contracts. Washington said that, as he understood it, the concept is to put the proceeds into a trust and to live off the interest. The funds certainly should not be used as an excuse for cutting back current funding for education.

Wright introduced **Karen Sollins** to speak on the Data Quality Act and its potential effects on DOE. The Act is part of a larger law passed at the end of the Clinton administration. Under it, each agency is to come up with a plan for assessing the quality of the data being provided to the public. According to a *New York Times* writeup, "It would create a system in every government agency under which anyone could point out errors ... . If the complaints were borne out, the agency would have to expunge the data from government Web sites and publications."

The Act was included in Section 515 of the Treasury and General Government Appropriations Act for Fiscal Year 2001. OMB then issued guidelines for ensuring and maximizing the quality, objectivity, utility, and integrity of information disseminated by federal agencies. In these guidelines, OMB offered these definitions:

- Quality is an encompassing term defined by utility, objectivity, and integrity.
- Utility is the "usefulness" to "intended users."
- Objectivity is "accurate, clear, complete, and unbiased."
- Integrity is the "protection of information from unauthorized access or revision."

There are more integrity issues than just security, however. Embedded in these definitions are some very hard problems.

Each agency is to (1) establish a basic standard of quality that is appropriate to the different categories of information disseminated; (2) provide a review process for quality prior to dissemination; (3) establish administrative mechanisms by which affected persons can seek and obtain appropriate, timely corrections. These guidelines are to go into effect on or after Oct. 1, 2002.

Each agency reporting must

1. designate a Chief Information Officer (CIO) responsible for this activity;
2. respond appropriately to any complaint;
3. report draft guidelines to OMB by April 1, 2002;
4. publish that draft in the *Federal Register*;
5. respond to comments and submit the final guidelines to OMB for review by July 1, 2002; and
6. report the number and nature of complaints annually.

This act and its associated guidelines raise several questions for ASCR. Does any data distributed by ASCR fall under this act? What are the criteria set forth for the evaluation of quality prior to dissemination? What will be the impacts be on the ASCR staff and the quality of ASCR data? What will be the impact of reporting? To what extent are the definitions achievable?

Washington commented that this Act slipped in with little scrutiny and is a very scary law. The release of data can be legally challenged and bottled up, making people reluctant to release their data and hampering the advance of science. Corones asked what it says about contractors. Sollins responded that it is not clear and reminded him that each agency gets to set its own standards.

Washington expressed the hope that the General Counsel's Office would make a ruling on whether DOE is subject to this law. Oliver noted that the first speaker on the next day's agenda is from the Chief Information Officer's office and might be able to provide insight on the issue.

Wright asked if people might use the Act to demand the removal of data from Web sites. Sollins

replied affirmatively and pointed out that ASCAC might be able to help DOE figure out how to walk through the maze and avoid any damage to ASCR's programs. Stechel commented that the American Chemical Society has looked at the problem, but she did not know if they have issued any statement.

Wright summarized the items to be dealt with the following day and called for public comment.

McCurdy asked about the Committee's response to Orbach's suggestion of a workshop on developing a plan for the future of scientific computing. Wright responded that the Committee has not organized the workshop yet but that Dahlburg has part of the answer. Dahlburg explained that a workshop is expected to be held in the following weeks and that it will be announced at the following day's meeting.

McCurdy asked what the strategy should be for SC to raise its budget for computational science. Wright said that the NSF panel that looked at computational science did not look at increasing budgets but at what work needed to be done, as driven by the science. McRae said that the tricky part is to make the scientific case for increased funding for computational science. Wright suggested that the Committee work on this issue, looking for some good science cases.

Stevens said that the NSF sought to get good testimony; there was a sense that a report would be produced that would influence the future of computing. He did not get the sense that ASCAC has been that engaged. There is already a budgetary envelope and strategy on the table that was not informed or influenced by this Committee. This Committee has to decide if it is going to be engaged or to comment from the sidelines. Wright agreed that the NSF effort was highly organized and that nothing that formal has happened in this Committee. She asked if the Committee wanted to assemble a similar type of panel to that brought together by the NSF. She noted that the Committee on its own cannot do that; it would need a charge letter from DOE management. Stevens asked if anything less would be effective. McRae said that, in his opinion, the question of having a formal panel is on the table. It could be suggested to Orbach; the Committee needs to talk with Orbach about what is the most important thing to do and have him write a charge letter. Wright observed that the Committee's current charge from him is quite narrow; the NSF effort was more than a year long and involved a great deal of staff support.

Giles commented that nothing the Committee does can influence the FY04 budget and asked how the Committee should respond to Orbach's question. Oliver noted that Orbach has to decide what to put forward to the Secretary to be pursued in the FY04 budget. If the Committee gives him any advice, it may influence what he proposes for the FY04 budget.

Wright asked whether the Committee should write a letter to him, meet with him, or do something else; she also noted that he had asked the Committee to respond. Sollins asked whether the Committee reported to Oliver. Oliver said, no; the Committee advises Orbach about the Office of ASCR.

McRae suggested that the Committee recommend a roadmapping activity for advanced scientific computing in SC be funded in the FY04 budget. SEMATECH (Semiconductor Manufacturing Technology) roadmaps could provide a good model.

Wright mentioned that the draft report of the NSF committee on cyberinfrastructure (on which she serves) is to be presented June 4 and asked whether that report will be able to influence the FY04 budget request. Oliver stated that it would be on the borderline. Wright continued that it is then almost too late for ASCAC to do anything to affect the FY04 budget. Oliver noted that the NSF's organization is less complicated than that of DOE, so June 4 is probably in time to influence its budget. Wright stated that the NSF committee on cyberinfrastructure is planning to recommend a substantial federal initiative in this area. She hoped that the NSF report is helpful in also making a

case for increased funding for ASCR to support a broad range of scientific efforts. Stevens called attention to the fact that DOE is complementing what NSF is doing in several places. That fact needs to be amplified and made known. Wright said that this could be done in a short time.

There being no further public comment, the meeting was adjourned at 5:38 p.m.

Friday, May 3, 2002

Wright called the meeting to order at 9:02 a.m. and introduced **John Pryzsucha**, Associate CIO for Cybersecurity of DOE. DOE now has a new CIO, Karen Evans. The office has reorganized and now reports to directly to the Secretary for both information technology (IT) and cybersecurity. The OMB says that DOE needs to do a better job of reporting its amount of IT and the management of that technology and it needs a capital-planning and investment-control process. This emphasis is partly being driven by the need to implement e-government, an unfunded initiative. Some of DOE's business-administrative systems and human-resources systems are currently duplicating other, existing systems. OMB is looking very hard at that duplication. The information side of DOE is very different from the science side. This type of reporting has a positive side and a negative side. The positive side is that the investment gives you visibility; the negative side is that you might need more money.

Giles asked if there was a precise definition of IT. Pryzsucha said that it was precisely defined in Form A-130. Giles explained that the Committee would be concerned if the NERSC computing facility were considered IT. Pryzsucha said that he would say that some IT supports NERSC but that NERSC itself is not IT.

OMB is pushing the envelope on what is reported as IT, but OMB is beginning to understand DOE's views about what is and is not IT. The Chief Financial Officer (CFO), deputy secretaries, CIO, and associate directors have formed a council to look over what is sent to OMB. Clinger-Cohen, the Information Technology Management Reform Act, says that DOE has to implement a process and make sure that there is an enterprise architecture. The program offices must develop a documentable, repeatable process for reviewing their investments, including IT. As a result, DOE is putting together a governance structure, and the program offices will develop a process that links to that governance. The Department will soon publish an enterprise-architecture document that will define its IT architecture and links that architecture to a capital plan.

Giles asked if they were tagging capital investments in just IT. Pryzsucha responded affirmatively, although, he pointed out, there is broader capital-investment tagging that covers other aspects. OMB gave a special training class on IT management for DOE, and several experts have been brought in to advise DOE on IT management.

Sollins pointed out that the Data Quality Act and OMB rules call for writing standards for data quality and for preparing for complaints from the public and asked what DOE has done along these lines. Pryzsucha responded that he had never heard of this law; it may be being handled by someone else. DOE might get some help from the System of Laboratories Computing Coordination Committee (SLCCC) to develop a unified response. Sollins went on to state that OMB has set criteria for accountability and has said that DOE (and virtually every other government agency) is at risk of losing funding.

Pryzsucha responded that DOE is working very hard on the management of its IT; this issue is quite urgent. A dialogue is ongoing between the DOE managers and OMB. Hitchcock said that DOE's policy is to document every computer-related system in the coming year.

Giles pointed out that there are several issues, including reporting major investments. DOE

should report such investments; this is not avoidable. But confusing scientific computing with IT *is* avoidable. DOE should make the case that scientific computing *is not* IT. Pryzsucha agreed that this distinction needs to be made, but also pointed out that the IT purchased to support that part of the infrastructure needs to be carefully reported. Wright asked if the CIO's office was working to make that difference clear. Pryzsucha responded that several CIOs [for example, of the National Nuclear Security Administration (NNSA), etc.] are working with OMB to that end. Giles asked what timeline they were working on and who is to make the decision of what is and what is not IT. Pryzsucha said that the program offices are to make that decision; the CIO is the facilitator between DOE and OMB.

Dahlburg asked what this Committee can do to get DOE off the "at-risk" list. Pryzsucha replied that DOE is not on any "at-risk" list; Hitchcock has filed the requisite documents to get it off that list.

Sollins asked what the view was of network routers and similar equipment that can have multiple uses. Pryzsucha responded that he appreciates the distinction but that it is not clear how to deal with dual-use equipment. There is, however, a method to separate the two types of equipment.

Wright pointed out that all of this equipment could get reported and DOE would get a great accounting score but would get no science done. She voiced concern about squandering money on reporting. Pryzsucha said that the program offices also have a responsibility for reporting; the CIO's office is trying to make some sense out of the process. This is a budget process, not a CIO process.

Wright called upon **Karen Sollins** and **Roscoe Giles** to talk about performance measurement. Sollins had looked at how different agencies do their evaluations, and Giles had participated in the BESAC Subcommittee on the Government Performance and Results Act (GPRA). Sollins had reviewed the processes followed by NSF, the Defense Advanced Research Projects Agency (DARPA), and the National Institute of Standards and Technology's Advanced Technology Program (NIST ATP), and had made use of the American Association for the Advancement of Science (AAAS) panel session on the subject at its 2002 meeting and OMB's report *Governing with Accountability*.

NSF uses two primary review criteria: intellectual merit and the broader impact. There are regular reporting and a final report to a program officer and reviews of larger programs. To meet GPRA requirements, NSF got approval to report "nuggets" in text rather than reporting numerically; the report to OMB states the effects of these nuggets. This encourages short-term projects. There are also regular visitations from a committee of visitors for each program.

DARPA is much more informal. Their criteria for evaluation are published in broad-area announcements. They perform an informal evaluation of technology transfer, and they keep in mind Heilmeier's criteria: What are you trying to do? Articulate your objectives using absolutely no jargon. How is it done today, and what are the limits of current practice? What is new in your approach, and why do you think it will be successful? Who cares? If you are successful, what difference will it make? What are the risks and payoffs? How much will it cost? How long will it take? What are the midterm and final "exams" to check for success?

NIST ATP is trying to cause new things to happen in industry. It initially peer-reviews projects. During a project, it conducts internal and external (contracted from the National Bureau of Economic Research) reviews. A study by the National Research Council found this process to be "an exceptional assessment effort."

The AAAS panel was a mix of professional evaluators and theoreticians. The professional evaluators said that evaluation is important and they rarely include peer review, although they sometimes include expert review. They never mentioned the impact of the evaluation process on the work being evaluated. One speaker from Europe reported less-than-stellar impact in most European

venues. They thought highly of GPRA, but then it was their jobs to do so. Evaluation may reflect a significant percentage of the cost of a program, so they recommended building the payment for evaluation services into the program budget.

To the academics, evaluation programs were not new, and they pointed to precursors to GPRA like zero-based budgeting and total-quality management. They used the phrase "utilization-based evaluation" to include:

- goal displacement (people will perform to the stated metrics);
- decisions in many of these processes preceding evaluation (there are many problems with the reporting period);
- the organizational burden associated with each of these processes;
- the problem of reporting failures in the research;
- the reporting process being only loosely connected (at best) to the political process of agency funding decisions;
- these reports' providing little insight into the process of an agency's priority setting; and
- the little connection all this reporting has to the larger question of national priority setting (one can make a good presentation and still not get any funding).

Governing with Accountability sets out five criteria. It seeks to:

1. attract stronger employees to government service,
2. expose tasks to competition to improve customer service while controlling costs,
3. improve financial management,
4. harness the power of the Internet to improve government, and
5. start the process of linking resource decisions to results.

Very little of this has to do with the question of how to set priorities among agencies and programs or with how to evaluate research. Nothing in the document asks whether good science is being done or whether an interesting agenda is being set. Instead, a scorecard is filled out every 6 months, and evaluation is left to an outside contractor. The report recommends legislation to allow (1) more management freedom within agencies and offices, (2) permanent reorganization authority, and (3) use of the scorecard to move programs from one organization to another. Concern was expressed at the AAAS meeting that moving programs might be done to punish agencies that do not meet with approval and could be done arbitrarily and without justification.

The conclusions that can be drawn from all this are:

- Metrics and evaluation are extremely difficult to do well.
- This is a political process that often does not match the decision-making process.
- The process can often have a significant impact on what is being measured and evaluated.
- Decision making may be very or even completely political.

Giles took up the presentation with a description of a workshop conducted by BESAC and attended by representatives from all the advisory committees in SC. The workshop was charged to review SC's current methods for measuring performance, the appropriateness and comprehensiveness of the methods, the effects on science programs, and the integration of performance measures with the budget process as required by GPRA.

The workshop was held in January and heard presentations from SC management, OMB, DOE's CFO, NIH, and NSF. The report was compiled, presented to BESAC, and approved. It recommended that SC

1. complete a Strategic Plan,
2. continue past good assessment practices (including peer and expert review),
3. align research evaluations with the Committee on Science, Engineering, and Public Policy

(COSEPUP) recommendations,
4. continue discussions with OMB about qualitative and quantitative criteria,
5. incorporate world-leadership criteria, and
6. include a goal of workforce development.

A prior strategic plan was not helpful in measuring and evaluating programs. But developing a strategic plan is a key part of the GPRA process. It is particularly important because its 5-year scope introduces a longer-term character into planning and 3-year, midcourse evaluations allow the introduction of new items into the planning process. Furthermore, a strategic plan's references to the Office's goals and the Department's missions provide criteria against which relevance can be measured.

Other comments on the recommendations include: For measuring research, the COSEPUP guidelines are very helpful and mostly reflect the use of peer and expert review. The discussions between SC and OMB should take into account the considerable qualitative component in measuring basic research and the long time scales involved. Assessment methods used by other, similar federal agencies should be considered to see if they might be appropriately used by SC. World leadership in all areas is not possible or even desirable. The maintenance of adequate human resources in fields critical to SC's missions should become a part of the evaluation process.

Several issues still remain: getting SC, OMB, and the CFO on the same page; developing a Strategic Plan for ASCR; setting comprehensive goals for the FY04 budget; and determining how good the metrics should be (the program descriptions in the FY03 budget request were truncated and not representative or comprehensible). Some "performance indicators" that were used in the FY03 budget request were "invited presentations at major national and international conferences," "software released to applications teams," and "percent unscheduled downtime." These indicators do not capture the scientific productivity; the number of science-facility users, the number of papers published, etc. may be better measures, but even these can be manipulated.

Stechel pointed out that these methods assume that only outcomes can be measured, whereas inputs can also be measured. This way of doing things raises the question of whether one is properly setting the stage for success. One can use leading indicators as well as retrospective indicators for success. For example, the Six Sigma process in industry looks at failures to getting the right outcome and develops a decision tree to get to the root cause of the failure. A quantitative measure can include scales of what resulted compared to what was expected. Giles responded that that was the thrust of the Subcommittee's recommendations, that there is a variety of ways to measure performance.

Connolly commented that peer review has to be incorporated into all measurements.

Wright asked if the Subcommittee had fulfilled its charge. Giles replied that the charge called for a report; that report was written, submitted to BESAC, accepted, and forwarded to the director of SC. The SC advisory committees can be involved constantly in helping the Office frame these measures. One hanging question is whether there is something that can be done to influence the FY04 budget.

Sollins asked if there was something this Subcommittee could do for ASCR. Dahlburg said that it might make suggestions about how to replace nonoptimal metrics. Sollins said that she would like to see some effective feedback to the program managers. Wright added that the Subcommittee could help make the criteria sensible.

Giles offered that the Subcommittee could circulate the recommendations of the COSEPUP reports. OMB has to agree to accept qualitative criteria, Sollins added, or scaled numeric data based on qualitative criteria. Giles noted that DOE's CFO and OMB are going to dictate how the

measurement is to be done.

Oliver pointed out that the advisory committees' weighing in on these issues is much more influential than the program offices' voice within the institution.

Wright stated that it would be desirable to have a proposal presenting criteria for evaluating basic research based on the COSEPUP criteria (world leadership, etc.) plus special provisions for the laboratories etc. that the advisory committee chairs could agree upon. She asked Sollins and Giles to draft something like that. Giles answered that he expected that a next-generation document will come from the advisory committee chairs in reaction to the Subcommittee's report. Wright said that she would contact the other chairs and tell them what ASCAC is doing. Those chairs are meeting with Orbach on June 3 and might be able to make some suggestions to him at that point.

A break was declared at 11:03 a.m. The Committee was called back into session at 11:33 a.m. Wright thanked the Office staff and the Oak Ridge Institute for Science and Education (ORISE) staff who make these meetings run smoothly. She introduced the issue of homeland security and asked the Committee's members to comment on their involvement in or knowledge of homeland security.

Stechel said that one issue is that homeland security needs pattern recognition, algorithms, threat recognition, and arrays of sensors. Dahlburg commented that visualization capabilities can be applied to sensor data; one has to display it, data mine it, etc.

Connolly called attention to the security needs of the nation's infrastructure and the need to make systems and middleware impervious to outside attack. Unfortunately, as one makes computers more secure, one makes them less open, an attribute that universities pride themselves on.

Giles pointed to the need for having reliable, redundant systems, ones that are stable and recoverable but open to the larger community.

Sollins called attention to the concerns of network security and privacy. These concerns arise just as the federal government wants to collect more information about individuals, information that they should not have, impinging on people's constitutional rights. What is happening is that people are just relabeling their work as homeland security.

Meza mentioned the need for simulations of critical-infrastructure (e.g., of the power grid), of bioterrorism acts, of the use of biosensors, and of the dispersal of biochemical agents. He also called attention to work being done on the design of foams for after-the-fact applications (e.g., for anthrax).

Lester mentioned the need for interagency communication.

Sollins said that, at the NSF, they felt the need to justify as many of their programs as possible as related to homeland security. If they don't do that, they will have their budgets reduced.

Wright commented that, at Bell Labs, an important issue would come up, management would say to the scientists, "What are you doing about it?", and there needed to be a reasonably fast answer. In this spirit, one could develop and analyze models of scenarios for homeland security. In addition, catastrophe preparedness needs human-computer interfaces to make the results meaningful to people in the field. Systems are needed that can make information immediately useful to people.

Kulsrud said that worries about openness are addressed in part by existing laws protecting mail, telephone, etc. The streaming of data presents a storage and mining problem; a workshop is being held on that topic next month.

Sollins called attention to a series of reports that have come out of a study that the National Research Council conducted on computer applications to catastrophe management. Stechel noted that the National Research Council is performing a decadal study on grand challenges for chemical engineering. They conducted a workshop in January; a report of grand challenges related to homeland security is coming out next month.

Wright called for public comment.

Sollins said that she would like to hear comments about metrics. In response, Hitchcock stated that evaluation is important. DOE has to figure out how to satisfy OMB, provide value to program management, and provide benefits to the research community. It is struggling to figure out how to tell the public what it is doing and why those tasks are important. Two possibilities might be helpful. (1) Develop serious roadmaps for facilities and activities that will be needed during the next decade. Facility, architecture, mathematics, computer science, and algorithm-development roadmaps could be drawn up. ASCAC could oversee their production or do them itself. (2) Figure out how to use those roadmaps as a basis for the other reports that OMB requires. Furthermore, in regard to homeland security, DOE has distributed facilities that researchers need remote access to. It needs to conduct research on trust models, group entrance, etc. That is a hard problem. Solving it would help them and us.

Meza said that the roadmap is a good idea. Wright asked if the Office has the time and resources to do this. Oliver said that doing roadmaps is part of the Office's normal business, and it is prepared to take on such a task. Hitchcock noted that the roadmap might produce items that would be useful in other tasks, like measuring performance.

Dahlburg commented that distributed sensors are like distributed elements on a computer, and whatever is done in mining and interpreting their data is also applicable to homeland security.

There being no further public comment, Wright adjourned the meeting at 12:05 p.m.

Prepared by
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Recording Secretary
May 25, 2002

Revised and submitted by
Margaret H. Wright, Chair
August 21, 2002