

**Final Minutes**  
**Advanced Scientific Computing Advisory Committee Meeting**  
**Feb. 27-28, 2007, American Geophysical Union, Washington, D.C.**

ASCAC members present:

F. Ronald Bailey	Horst D. Simon
C. Gordon Bell (Tuesday morning only)	Ellen B. Stechel
Jill P. Dahlburg , Chair	Rick L. Stevens
David J. Galas	Virginia Torczon
Roscoe C. Giles	Robert G. Voigt, Co-Chair (Tuesday morning only)
James J. Hack	Thomas Zacharia
Thomas A. Manteuffel	

No ASCAC members absent

Also participating:

Melea Baker, Office of Advanced Scientific Computing Research, Office of Science, USDOE

David Brown, Office of Advanced Scientific Computing Research, Office of Science, USDOE

James Coronas, President, Krell Institute

Barbara Helland, Office of Advanced Scientific Computing Research, Office of Science, USDOE

Daniel Hitchcock, Senior Technical Advisor, Office of Advanced Scientific Computing Research, Office of Science, USDOE

Gary Johnson, Office of Advanced Scientific Computing Research, Office of Science, USDOE

Frederick M. O'Hara, Jr., ASCAC Recording Secretary

Raymond L. Orbach, Under Secretary for Science, USDOE

Walter Polansky, Office of Advanced Scientific Computing Research, Office of Science, USDOE

Michael R. Strayer, Associate Director, Office of Advanced Scientific Computing Research, Office of Science, USDOE

David Thomassen, Chief Scientist, Office of Biological and Environmental Research, Office of Science, USDOE

Christopher Yetter, ASCAC Designated Federal Officer, USDOE

About 30 others were in attendance.

**Tuesday, February 27, 2007**

**Preliminaries**

Chairperson Jill Dahlburg called the meeting to order at 9:00 a.m.. She welcomed the four new committee members and had all the members introduce themselves. Rick Stevens has agreed to be the Cochair of the joint subcommittee with the Biological and Environmental Research Advisory Committee (BERAC). Chris Yetter announced that the next meetings will be on August 14-15 and November 6-7.

## **Michael Strayer: View From Washington on the Office of Advanced Scientific Computing Research**

In budgets, the first surprise was the FY07 request for ASCR, a 33% increase over the FY06 appropriation of \$228.4 million. The second surprise was that Congress agreed. However, the continuing resolution nullified this increase but still resulted in a substantial increase over the FY06 appropriation. The budget of the Office of Science (SC) is known and fixed, but the distribution of those funds across the program offices is not. The FY08 request for ASCR is for \$347.7 million, which will allow a continued buildout of ASCR's core program in applied mathematics and allow ASCR to address critical long-term mathematical research issues relevant to petascale science, multiscale mathematics, and optimization control and risk analysis in complex systems. The Computer Science Graduate Fellowship is being built out with a \$1 million increase to \$5 million. ASCR will also develop software and tools to enable researchers to use petascale systems at the leadership computing facilities (LCFs) and supercomputing facilities. ASCR will focus on accelerated visualization, uncertainty, user interfaces, and low-power-density approaches to petascale computing.

SC has established a common platform to evaluate all national laboratories against the same goals, objectives, and statistics. This new system will be more fair and consistent.

ASCR underwent a reorganization this past year with the introduction of four (*is this two, not four?*) new divisions. The Computational Science Research and Partnerships Division (SciDAC) now has groups in Applied Mathematics, Computer Science, Partnerships, and Distributed Networked Environment. The Facilities Division now has groups in Facilities and Operations.

Recently, ASCR has held three workshops: (1) Mathematics Research Challenges in Optimization of Complex Systems, (2) Computational Subsurface Sciences, and (3) DOE Cybersecurity R&D Challenges for Open Science. Future ASCR workshops will be on computational science and engineering, cybersecurity research needs, applied mathematics research, mathematics for large data set analysis, and computational science research needs in alternative and renewable energy.

In the buildout of ASCR facilities, the Argonne Leadership Computing Facility (LCF) will install the 100-teraflop IBM Blue Gene/P, the Oak Ridge Cray XT3 was upgraded from 25 to 54 teraflops with a 100-teraflop upgrade in final acceptance testing, the National Energy Research Scientific Computing Center (NERSC) 100+-teraflop Cray XT4 was delivered, and ESnet has completed its second and third metropolitan area networks to provide dual connectivity at 20 Gb per second for the Large Hadron Collider (LHC) Tier-1 data centers and signed a major partnership agreement with Internet2. The INCITE program [Innovative and Novel Computational Impact on Theory and Experiment] is enabling science with supercomputing through traditional, transparent, peer-review processes. 95 million processor hours were allocated to 45 projects. The national plan for advanced networking research is now an Office of Science and Technology Policy initiative with Daniel Hitchcock as co-chair.

**Discussion:** In the applications for INCITE, there was a difference of about 240 million hours between the old and new proposals. The two-phase review was comprised of a computational readiness review and a scientific review.

## **Raymond Orbach: Presentation from the Under Secretary for Science**

The 2007 budget will go to the Office of Management and Budget (OMB) a few days after this meeting and to Congress in mid-March. SC is working on the FY08 and FY09 budgets. The

role computation plays in the nation's competitiveness and in global climate change shows up directly in the President's budget. The FY08 budget focuses on three themes: transformational science, national scientific facilities, and a skilled scientific workforce (SC supports >25,000 researchers, faculty members, and students in the United States).

FY06 was a difficult year, unfunding thousands of researchers. SC received significant increases in FY07 but still short of what the President requested. SC will ask for a \$600 million increase in FY08 over the FY07 enacted. That will get SC back on the doubling trajectory. But SC still lost \$305 million in FY07.

The ASCR budget shows an extraordinary 49% increase from FY06 to FY07. That is a statement of trust, and a responsibility. ASCR is a major player in SC. These results come from ASCAC's advice. These increases will bolster core research to incrementally bring that funding back to parity with facilities funding. It will take five years of increases to recover from 15 years of flat budgets. The increase in SC's FY08 requested budget will be \$776 million.

There is a concern that federal agencies are too conservative in research funding. There are pressures to fund high-risk, high-potential-payoff research. The way SC addresses this concern is to hold workshops to think innovatively and transformationally. This is how new ideas are funded, researched, developed, and introduced to industry.

In facilities, three bioenergy research centers have been granted \$375 million over 5 years, buying down the risk capital to entice venture capital to come forward to support basic research. The National Synchrotron Light Source-II (NSLS-II) is in the design stage now. The Linac Coherent Light Source (LCLS) is under construction. The Spallation Neutron Source (SNS), a \$1.4 billion machine at Oak Ridge National Laboratory (ORNL), was built on time and under budget, restoring the credibility of DOE before Congress and the world. All five nanoscience research centers will be open to all this year. The advanced computer science centers are extending the frontier of science, and by the end of 2008, SC will have petaflop computing in Oak Ridge. The Tevatron and B-Factory are compiling data at an incredible rate.

SC intends to increase the inspiration of America's youth with DOE Academies Creating Teacher Scientists (ACTS) and the National Science Bowl for High School and Middle School Students. In INCITE, industry is learning from DOE how to manage and support large-scale computing projects.

**Discussion:** DOE has identified 28 areas that could benefit from robust support for applied science. The workshop on nuclear energy last summer is an example. It asked, can one simulate a nuclear reactor from atomic to macro scales? That is a tremendous challenge. ASCAC has an opportunity to point out such opportunities for a great many applied sciences and technologies. SC has the facilities and expertise to address these problems.

The INCITE process is international. Julich will be the high-end computer center for Germany. They expect industry to contribute support. Grid computation has been the focus of European research; they are looking at other approaches now. Often, other countries buy big machines that just sit there. The Earth Simulator's lack of remote-access capabilities limited the utility of that machine. Collaboratories and networking need to be encouraged.

A break was declared at 10:50 a.m. The meeting was called back into session at 11:03 a.m.

### **Gordon Bell: Report Discussion on Charge 1, Performance Metrics for Computational Facilities**

Dr. Orbach's 10 MAR 2006 charge to the ASCAC, on the topic of science-based performance metrics, was parsed into six items: (1) performance measurement and assessment,

(2) the appropriateness and comprehensiveness of the measures, (3) computational science component of the science accomplishments, (4) effects on SC's science programs, (5) evolution of the roles of these facilities, and (6) computational needs over the next 3 to 5 years.

The centers have four control metrics for measuring performance: user satisfaction, scheduled availability, response time to solve user problems, and support for high-capability work at the leadership computing facilities. One can also use a large number of observed metrics: user sophistication, level of support, scheduled and overall system uptime, use of centers' resources, use of standard and specialized software, individual project metrics, individual project scalability and efficiency on each platform, use of software tools, workflow management, and productivity. Many things can be observed, but only a few can be used to control.

The Subcommittee supports a goal of halving the time to solution every 3 years.

Science accomplishments can be measured with publications, codes and data sets, people, technology transfer, project milestones, exploiting parallelism and/or improved efficiency, and breakthroughs (which can only be measured retrospectively).

A clear process should be implemented that measures the use and effects of the computational resources on the projects within each SC office. Each office should report the total investment in all projects, using a rough conversion of computer time to dollars. The process of allocating computer time at the centers through the program offices should be re-examined in light of the diversity of architectures.

**Action:** Dahlburg asked each member to assess the report. All the members of the Committee present (Voigt had left) accepted the report with no modifications beyond those mentioned in the presentation. Dahlburg said that she would draft a cover letter and forward the report to Orbach as amended and voted-on by ASCAC during Bell's presentation.

**Additional Discussion:** To make the value of computer time more significant, ASCR could put the computer time in dollar figures to outside clients; there could be an analog to how facilities allocate resources. A facility's systems should have a strong tie-in with the projects using them, and DOE should be more of a partner with the users. The difficult problem of measuring scientific understanding and accomplishments needs ongoing study, and the impacts of the implementation of any of the Subcommittee's recommended objectives should be monitored.

### **Daniel Hitchcock: Management Principles for High-Performance-Computing and Leadership-Computer Acquisitions**

The computing centers are large investments. Weak investments in the past have resulted in leveraged systems that were liabilities. Some procedures to work from were needed. The basic rules of thumb are: do no harm, use extant processes that work, make sense, use peer review, and build bridges to the applications communities (e.g., to the biological community).

DOE Order 413.3: Project Management has to be followed. It calls for a formal five-step process for managing projects, including external reviews.

In collaboration with the Office of Biological and Environmental Research (BER), ASCR has tailored some project-management principles, tested those principles, and documented the comments of reviewers. Each upgrade project is to have a project-execution plan (containing the roles and responsibilities, baseline, financing plan, etc.), acquisition strategy, and acceptance plan. The project phase terminates at the acceptance of the computer. Upgrade projects also have transition-to-operation plans, but these are not part of the project.

**Discussion:** All of this procedure is working for the LCFs, and part of it is working at NERSC. Daniel Lehman had conducted reviews of the LCFs, and reviews of the rest of SC are being performed. When all of the money is going into large acquisitions, earned value management is not an optimal tool, but its use is mandated; it shows if money and schedule are in alignment.

### **Ellen Stechel: Report Discussion on Charge 2 – Examine the Role and Efficiency of Networking and Networking Research within SC**

The Subcommittee for Dr. Orbach's 10 MAR 2006 to the ASCAC, on the topic of the role and efficiency of networking and networking research within the SC, was asked to weigh and review the organization, performance, expansion, and effectiveness of the current operations of ESnet; consider the proposed evolution of ESnet; and make suggestions and recommendations on networking research. The primary focus is on 5 to 10 years out.

The Subcommittee needs clarification on (1) the initial sentence of the charge, especially in light of the Lehman review that found ESnet to be effectively managed and responsive to its customers and to DOE program management; (2) how to address unforeseen future technology options; and (3) the principal drivers that led to the charge.

The Subcommittee hopes to produce (1) useful guidance on networking research, the evolution of the network, and strategic relationships; (2) the priority of networking needs; (3) a vivid picture of how the network might be used 10 years hence and a strategic vision of a new generation of networks and globally distributed systems; (4) how science will be practiced in the future and how networking will enable the advancement of science; and (5) leveraging of the private sector. It also expects to have findings on setting the standard in data and information management, technology gaps, security and its relationship to science applications, end users and other stakeholders, and productivity or effectiveness measures.

The Subcommittee held its first teleconference in February 2007 and is continuing to meet biweekly. It will visit ESnet in April, issue a status report in August, distribute a draft preliminary report to ASCAC in October, and deliver a final report in January 2008.

**Discussion:** Firewalls and cybersecurity are being considered. Opportunities in collaboratories would be looked at, and there is a person on the Subcommittee with that expertise.

### **Gary Johnson: Sub-Surface Modeling**

The Computational Subsurface Modeling Workshop, 9-12 JAN 2007, was a collaborative effort of four DOE offices: SC, Environmental Management (EM), Fossil Energy (FE), and Civilian Radioactive Waste Management (RW). The workshop charge included identifying computational science research needs and opportunities in the subsurface sciences and related areas, assessing potential terascale computational algorithms to enable high-fidelity subsurface simulation models, and preparing a report.

More than 150 registrants representing many disciplines came from 11 national laboratories, 25 universities, a sprinkling of industries, and DOE headquarters. The workshop final report has not yet been submitted. Cross-cutting topics and challenges were uncertainty analysis, new multiscale computational tools, high-fidelity simulations, and increased collaboration. One point that came across is that researchers feel that they work too much in isolation. Collaborative efforts need to be put together.

Approximately 17 proposed research directions were identified. Conclusions drawn by the workshop: The computational subsurface sciences research agenda challenges the limits of current simulation capabilities. Many opportunities for significant advances in simulation capabilities and mutually beneficial collaborations exist. The daunting challenges related to the multiscale, multi-physics nature of subsurface sciences need to be addressed. Collaboration will be required between discipline scientists in the DOE application offices and computational scientists in SC's ASCR.

### **Walter Polansky: Update on SciDAC**

*Scientific Discovery*, a progress report of the SciDAC program, was published. The number of publications from the program increased from 94 in 2001 to 377 in FY06. Recent successes include raising the efficiency of codes by more than 10,000% and a 2006 R&D 100 award for the data-mining tool Sapphire.

The goals of SciDAC-2 are to create a comprehensive, scientific computing software infrastructure to enable scientific discovery across a broad spectrum of sciences at the petascale and to develop a new generation of data-management and knowledge-discovery tools for large data sets.

On September 7, 2006, SC announced approximately \$60 million in new SciDAC annual awards for 30 computational-science projects over the next 3 to 5 years. SciDAC is a \$61.5 million program, with \$29 million going to 18 applications, \$24.3 million to 9 centers, and \$8.2 million to 4 institutes. New faces make up about 60% of the SciDAC-2 funds. SciDAC participants represent 17 laboratories, 55 universities, and 3 companies. The same review standards are used for all proposals. ASCR provides \$41.3 million of the funding with the rest coming from other DOE offices and federal agencies. This is a resounding success for SciDAC-1.

The Institutes are university-led centers of excellence that focus on major software issues, employ a range of collaborative research interactions, reach out to engage the broader community of scientists in scientific discovery through advanced computation and collaboration, and conduct training/outreach in high-performance computing topics. The Centers for Enabling Technology (CETs) are chartered to work directly with a suite of applications. They will enable scientific simulation codes to take full advantage of tera- to petascale machines, ensure critical computer-science and applied-mathematics issues are addressed in a timely and comprehensive fashion, and address issues associated with the research software lifecycle. SciDAC challenges: provide a fertile environment for scientific discovery through modeling and simulation; make SciDAC resources available to the broad research community; communicate the SciDAC model; and, optimize relationships among CETs, applications, and institutes. The SciDAC Outreach Center is primarily an interface for someone who is computationally cognizant in high-performance computing but outside of DOE. This center has innovative web and software services and conducts workshops and training sessions to build collaborations to drive a scientific discovery.

Two solicitations have been issued; the Climate Change Prediction Program notice, which closed January 25, 2007; and, a solicitation on accelerator science and simulation that was released by HEP, NP, BES, and ASCR, which closed January 17, 2007.

In June, SciDAC will hold a scientific conference on high-performance computing in simulation in Boston.

**Discussion:** An annual call for participants will not be issued in 2007, just the limited solicitation. For FY08, the line item is blank. Reviews will be conducted to see if application needs are still being met by SciDAC projects. Asked if there is validity to the concern that SciDAC-2 had turned toward short-term software development, Polanski said that he did not think it was a valid observation. The FY08 budget has a major increase that enhances base research. The focus on collaborative groups has not been lost. Collaboratories filled a meaningful niche in SciDAC-1; in SciDAC-2, one collaboratory was the open-science grid and the other was in climate change.

### **David Brown: Strategy for the Applied Mathematical Sciences (AMS) Program**

The AMS program was begun in the 1950s. It has resulted in models, analysis, and algorithms for partial differential equation (PDE) based science, such as theory and numerical simulation of PDEs, fundamental stability and accuracy of difference methods for PDEs, numerical methods for shock physics, scalable methods for solving large systems of linear and nonlinear equations, and other areas. Software was provided to users through robust math software libraries, which have a crosscutting impact on multiple science and engineering applications.

Today's SciDAC discoveries are enabled by past base-program research. Modeling and basic algorithm research have led to prototypes and proofs of principle that bred hardened science-application codes. This is a model that has worked in the past. The question is, what do we need to do to ensure that the AMS program is as successful for the next 50 years as it has been for the past 50?

One needs to get past the view that applied math is a "support" discipline for other sciences. As new opportunities emerge, the AMS program's emphasis must adapt, putting increased emphasis on scientific data understanding at the high end for both simulation and experiment. Models for man-made systems will involve new types of math, such as coupled discrete and continuous models and nonlinear effects.

In the near term, we will propose new math initiatives for FY09 and FY10 to infuse increased funding and new ideas into the AMS program. In the longer term, we will develop an AMS strategic plan, engage the DOE math community, get input from scientists knowledgeable about the DOE mission and programs, and leverage the National Research Council study that makes the science case for computation. This plan will articulate 10- to 20-year goals for the AMS program and to map out 5-year strategies for achieving those goals. A Computer Science Graduate Fellowship (CSGF) for applied mathematics is needed. One could apply the CSGF model to the early-career principal-investigator (PI) program. Laboratory internships for undergraduates and graduate students should also be promoted. We will encourage collaboration and communication, and AMS must effectively leverage academic expertise.

**Discussion:** Asked if there will be a catalyst for reestablishing the sense of community, Brown responded that the sense of *common purpose* was a unifying force. He had not thought about how to reinforce a sense of community. Some *problems* are unifying influences, like Genomes to Life (GTL). One challenge is how to have continuity over a 50-year timeframe. Applied mathematics can be curiosity driven, but now things are 3-year-project driven. One must have a long-term vision while navigating the bureaucratic minefield; this duality is very important. Many new math areas may need new computing models and platforms. AMS has always been doing multiscale math, but just did not call it that. Multiscale math is basic to the

mathematics program. An applied math program should be closely tied to high-performance computing; otherwise, these systems will go unused.

### **Administrative Issues**

Yetter said that there should be three Committee meetings next year. One should be at about the same date as this meeting. Dahlburg suggested that they be held at the same times as the meetings of this year. Yetter said that he would e-mail the proposed dates to the Committee members on the following week. Bailey asked about locations. Yetter said that the February meeting should be held in Washington, D.C., so that the Under-Secretary could attend. We should hear about other locations soon.

Dahlburg called for public comment. There being none, she adjourned the meeting for the day .

**Wednesday, February 28, 2007**

### **Michael Strayer: New Charges – COV Review of Computational Partnerships and Joint Panel with BERAC**

On August 15, 2003, ASCAC was charged to institute a committee of visitors (COV) to assess the program management of major elements of ASCR. Previous COV reviews of selected research programs and facilities were very successful. Now, a COV review of SciDAC is needed. SciDAC is more than 5 years old and has offered two solicitations. This COV will touch upon partnerships with other DOE offices that entail \$60–70 million as well as other ASCR-based programs. The report will be due for the ASCAC Fall 2007 meeting, and Robert Voigt will lead this COV.

In addition, we need to convene a joint panel with BERAC to examine the issue of computational models for GTL, how progress could be accelerated through targeted investments in applied mathematics, and how computer science can be incorporated to meet the needs of computational biology. The joint panel should consider whether the current ASCR long-term goal is too ambitious, given the status and level of buy-in from the community. It needs to consider what is happening in the computational-science and life-sciences communities. It should discuss possible intermediate goals that might be more relevant to the two programs. And it should identify the key computational obstacles to developing computer models of the major biological understandings necessary to characterize and engineer microbes for DOE missions, such as biofuels and bioremediation. An interim report will be due in May 2007 (to discuss issues per OMB), and a final report will be due in August 2007. Rick Stevens has offered to lead this effort.

**Discussion:** The final report of the joint panel will have to be accepted by both ASCAC and BERAC. If the Subcommittee has made significant progress, the “final” report may be accepted at the May BERAC meeting.

### **Gary Johnson: DOE Cybersecurity R&D Challenges for Open Science Workshop**

The workshop was held in North Bethesda on January 24–26, 2007. It was charged to identify the research needs and opportunities associated with cybersecurity for open science; to focus particularly on those needs associated with DOE supercomputing, user facilities, high-speed networks, national laboratories, and other open collaborative science stakeholders; and to discuss how open science cybersecurity differs from general cybersecurity.



The 55 registrants came from 14 national laboratories, 8 non-DOE organizations, and DOE headquarters. The workshop identified four proposed research directions: (1) multi-site situational awareness and response; (2) managing authentication and attribute-based authorization; (3) software, data, and systems assurance; and (4) cybersecurity policy specifications. Groups are working on each of these topics but are working separately; their efforts should be coordinated. The workshop came to the following conclusions:

- The diversity, heterogeneity, and scope of the open-science environment bring unique cybersecurity challenges.
- Software for modern open science is not available from commercial sources.
- The high-performance environment, local user population, and diversity of custom applications and software in the open-science environment make protecting the facilities and detecting malicious attacks uniquely challenging.
- The expertise and tools developed in a cybersecurity research program for open science would have a broad impact and would establish SC as a leader in cybersecurity in the wider community.
- Additional effort is required to adequately define cybersecurity's priority research directions.

The final report has not yet been prepared. In collaboration with DOE's Office of Electricity Delivery and Energy Reliability (OE), SC is planning a follow-up workshop.

**Discussion:** Doubts were expressed whether the requirements were self-evident. The task is seen as a path of discovery. The disjoint between OE (an applied office) and the research to be identified and done is only an apparent one; OE's involvement will not necessarily be in applied technology. Whether the second workshop will be specifically charged to identify needed R&D is unknown as the charge has not yet been written. There are many formats for workshops that can elicit useful information, and new processes are being developed collaboratively with other offices. On this path of discovery, lessons learned should be tracked.

In regard to cybersecurity's importance to ASCR and its budget, it was pointed out that there is an expectation that an initiative will follow the workshop(s). A plan for cybersecurity should result from the results of this workshop. It was suggested that this Committee should discuss how much security (and burden on the user) is appropriate. In response to a question about what the basic research in cybersecurity was, Johnson agreed to provide some examples.

### **James Coronas: Outreach and Communication Project for ASCR**

This effort started in earnest about eight months ago to communicate clearly and crisply the value, importance, and world-class quality of the facilities, research, and people supported by ASCR. The audiences for this information are decision makers, technical communities, and the interested public. The media and the public are generally not cognizant of DOE-supported research. Moreover, joint funding of many activities dilutes or hides DOE's role.

Purposes include: to create a broad range of accessible materials that communicate to wide but selected audiences; to make these materials widely and easily available to the target audiences; and, to organize and archive this material for multiple use in multiple forms. An editorial board has been established to suggest exciting topics. The first product is *ASCR Discovery*. The design, contents, and structure of that online publication will evolve, and other modalities will be developed. Comments and ideas on this project will be welcome.

**Discussion:** Asked how the Krell Institute's involvement in the SciDAC review will interact with this effort, Coronas replied that the information will be linked but the efforts will be

separate. In regard to getting this product read by the main target, decision makers, problems with distribution need to be grappled with, and contact needs to be made with the scientific writing community and the media. This project will also address the long development time of some projects. It is critical to tell some of these stories.

### **Virginia Torczon: Workshop on Mathematical Research Challenges and Optimization and Complex Systems**

The goal of the workshop was to articulate opportunities for mathematical research relevant to DOE applied science and technology programs, particularly mathematical areas that do not currently constitute a major fraction of DOE's applied mathematics research portfolio. The workshop focused on complex systems, optimization, risk, and control. It had four plenary talks (on optimization of fossil-fuel power generation, the nuclear-fuel lifecycle, power-grid control and optimization, and risk assessment for cybersecurity) and five cross-cutting breakout sessions (on networks and stochastics, complex systems and statistics, control and optimization, model construction and validation, and risk). The workshop was to look for areas where investment in mathematics and simulation and modeling might provide big payoffs. Six areas were identified:

- Effective modeling of heterogeneous, coupled, human-made systems with nonlinear interactions;
- Analysis and algorithms for a variety of optimization problems involving large systems with a large mixture of continuous and discrete variables;
- Methods for analyzing and responding to sensitivity in highly nonlinear systems;
- Statistical approaches for validating and improving mathematical models of nonphysical systems with a limited number of observed data;
- Techniques for developing, validating, and integrating computational models with real-time data to support decision making and adaptive control; and
- Careful analysis of how risk should be incorporated into complex-system models.

There are strong intersections among the six mathematical areas identified by the DOE workshop and research needs identified in other recent SC studies. These are challenging research areas that will require a sustained long-term investment. DOE is not the only one looking at this subject.

**Discussion:** The aerospace industry has been facing these problems for decades; DOE should actively consider what is happening outside of the Department. The scale of needed investments has not thought about, yet. Scientific opportunities need to be balanced against technical opportunities, and one has to have sufficient structure to make it worthwhile and usable. This task has been a recognition of gaps, since not a lot of money has been going to modeling. One way to look at it is that these are very difficult problems, and there need to be investments for both mathematics and the applications. One needs to step back and reformulate the problem in terms of algorithms and models which can only be done by involving mathematicians and bridging the communication gaps.

**Action:** Dahlburg called for public comment. There being none, she adjourned the meeting.

Respectfully submitted,  
F. M. O'Hara, Jr.  
Recording Secretary  
Mar. 23, 2007