Final Minutes
Advanced Scientific Computing Advisory Committee Meeting,
Nov. 8, 2006, Marriott Washingtonian Hotel, Gaithersburg, Md.

ASCAC members present:

F. Ronald Bailey, Acting Chair
Gordon Bell
Roscoe C. Giles
James J. Hack
Ellen B. Stechel
Virginia Torczon

ASCAC members absent:

Jill P. Dahlburg , Chair
David Galas
Thomas A. Manteuffel

Also participating:

Melea Baker, Office of Advanced Scientific Computing Research, Office of Science, USDOE
Frederick O'Hara, ASCAC Recording Secretary
Rick Stevens, Director, Mathematics and Computer Science Division, Argonne National Laboratory
Michael R. Strayer, Associate Director, Office of Advanced Scientific Computing Research, Office of Science, USDOE
Christopher Yetter, ASCAC Designated Federal Officer

About 15 others were in attendance.

Tuesday, August 8, 2006

Preliminaries

Acting Chairman Ronald Bailey called the meeting to order at 9:50 a.m. and reviewed the agenda, which consisted of considering two subcommittee reports recommending PART [Program Assessment Rating Tool] program scores that must be provided to DOE by the end of November for submission to the Office of Management and Budget (OMB). Michael Strayer thanked the Committee for its diligence in completing these important reviews on such short notice. Christopher Yetter announced that the next Committee meeting will be Feb. 27-28, 2007.

Virginia Torczon: PART Evaluation of the Genomics:GTL Program

The Subcommittee was asked to evaluate the progress of this program toward its long-term goal. Measures of the grades Excellent, Good, Fair, and Poor were developed in cooperation with the Office of Biological and Environmental Research (BER) and its advisory committee (BERAC). The Office of Advanced Scientific Computing Research (ASCR) is co-funding projects in the GTL program and has also made awards through the life-sciences portion of Scientific Discovery Through Advanced Computing (SciDAC). In addition, ASCR has created three institutes for the advancement of computational biology to serve the broad life-sciences community (as well as GTL) by training future researchers.

There has been active cooperation with BER, biologists are involved in reviews, the institutes are active, and efforts are being made to better integrate computational biology into life-science activities. Interdisciplinary research is being fostered by eliminating

barriers posed by inadequate communication and disparate timescales for achieving research objectives. Adequate communication exists with BER but not necessarily with the broader biological community.

BERAC was asked not only to grade progress but also to consider the appropriateness of the measures. In response to a National Research Council (NRC) review and a change in administration policy, BERAC recommended modifying both the charge and the long-term measures, adding the study of plants and the production of biofuels to the characterization of multiprotein complexes and the development of computational models of microbial communities. Another subtle difference in the long-term measure is that the BER version does not mention cooperation with ASCR, whereas the ASCR version specifically mentions that the work is done in cooperation with BER. Also, the new grade definitions refer to a "systems-biology understanding," raising the question of whether this adds more biology and means less computational modeling.

Given these new definitions, it is not clear that the new long-term goal can be met by 2015, so the ASCR Subcommittee was reluctant to give a grade of Excellent, as was recommended by BERAC.

Discussion: It is unclear whether the management structures are in place to cover the increased scope of the GTL program. More important is getting computer science into the program and its institutes. DOE can make that happen. The modeling effort has to be multidisciplinary, and the institutes are a good way to do that. Both SciDAC projects are based at national laboratories, making that multidisciplinary effort easier. No overall roadmap is evident. It seems that new projects focus on new libraries or species. Tool-development efforts are under way to get better results. Also needed are getting other disciplines involved, validating, and re-engineering. The strength of the three institutes is in the biology; their computer science is not at the cutting edge and needs to be upgraded. The work funded by ASCR has computer-science contributions (e.g., rapid-workflow programs); on the BER side, there *is* similar work being done, but it is too early to see results.

Public comment: There were many workshops identifying the community, drawing up roadmaps, and addressing a lot of issues over several years. ASCR has not had a budget to engage this problem. If the best modelers were involved, BER would not overlook a problem. Programming would be better served by aggressively addressing the problems.

A message about these concerns should be sent to DOE by voting to accept this report at this meeting and adding comments. Given the limited funding, this is an excellent start; but given the low funding, this is only a good effort to achieve the long-term goal. Money would always help in making it excellent. However, it is not just an ASCR issue, and that makes it a difficult situation. The report should say this is a good program and that improvement is expected as the biology and computer science communities get to work together. BER and ASCR should work together, looking at this report after it comes out. The reinterpretation of the question by BERAC leads to skepticism about whether the long-term goal can be met and indicates a lack of collaboration between ASCR and BER.

Action: A break was declared at 10:47 a.m. to draft a concise statement of the concerns. The meeting was called back into session at 11:04 a.m. The statement of concerns read: "Our PART grade of Good reflects a judgment of the progress toward

validated computational models by 2015. This progress depends essentially on effective integration and collaboration of biological and computational research efforts. We judge ASCR's contribution and progress in the context of resource constraint to be excellent." The grade of Good is on the overall effort. The solution of the problem is beyond the scope of ASCR.

A vote was called for on granting a grade of Good. The vote was five in favor with one abstention. The word "outstanding" was substituted in the statement of concerns for the word "excellent" to avoid confusion with the grade of Excellent.

Ellen Stechel: Evaluation of Modeling of Complex Systems

The Subcommittee was asked to evaluate progress toward the long-term goal of developing mathematics, algorithms, and software that enable effective scientifically critical models of complex systems, including highly nonlinear or uncertain phenomena or processes that interact on vastly different scales or contain both discrete and continuous elements. It found that ASCR has made an excellent start toward achieving the goal of enabling effective modeling of complex systems, in particular those systems with processes that interact on vastly different scales.

ASCR has initiated two key efforts to address this long-term goal: one focused on advancing multiscale mathematics to address processes that interact on vastly different scales and one addressing the broader set of mathematical challenges in the field of complex systems. A workshop is scheduled for December 2006 on mathematical research challenges in optimization of complex systems; it will address the broader set of issues beyond multiscale mathematics, which is necessary to fully address the long-term goal.

This whole effort was initiated in 2004 with a series of three workshops that defined the opportunity and a path forward. An important conclusion of those workshops was that the multiscale challenge will not be advanced solely by increasing capability computing but will require the development of new mathematics, new algorithms, and collaborations among domain scientists and mathematicians.

ASCR funds a Multiscale Mathematics Research and Education Program, which issued a request for proposals in 2005. Thirteen proposals were funded from the 170 received (<8%), with awards ranging from $650,000 to $2.6 million and covering biological systems, plasma physics, nanoscale materials, and climate systems. The researchers are making good progress.

The Subcommittee concluded that the multiscale mathematics program needs to grow; its first opportunity for new proposals will be in FY 08. Mathematical research challenges in optimization of complex systems will require new funding if ASCR is to continue to make progress toward the long-term goal. At the same time, the portfolio breadth of the Office's core applied and computational mathematics needs to be maintained. Finally, growth in these mathematics programs should not fall to a lower priority than investments in hardware to achieve petascale computing because mathematical and algorithmic advances are absolutely necessary to address the modeling challenges in complex systems and, therefore, to meet the long-term goal.

Discussion: Asked about the advances that will be made, program managers said that these are new projects that raise basic issues. Spectacular results should not be expected at this early stage. These efforts will likely change how problems are solved, particularly

in materials science, and, by extension, how materials are used in all industries. They will show how and why advanced and hybrid materials fail, which would be an important advance in knowledge. One needs seamless mathematical formulations while crossing the different scales from the micro to the macro to do this. New mathematics will be needed and would have broad application. Multiscale mathematics is an enabling capability in addressing many problems of critical interest to DOE's mission. The length and time scales cannot always be separated; advances require less brute force and more mathematics fundamentals.

Whether or not U.S. multiscale computing is world-class varies from topic to topic. General principles are involved, and the crux will be to find those principles. This program is experiencing an excellent start, but it has a long way to go. The researchers are very early in the process, having gotten started on pieces of several complex systems. It *is* progress; however, the goal is not written with enough specificity to know when it has been achieved. Progress will be observed as developments are made in mathematics and algorithms and as those developments are used to solve important problems in science.

Only 8% of the Multiscale Mathematics Research proposals were funded; 10 to 30% could be funded if money were available. Funding sets the bar. The program also has the indirect effect of raising the visibility of this whole area. There were many excellent proposals submitted but not funded. For many years, great mathematicians were located in Moscow, Russia. Many of those mathematicians have diffused to the West and will make great contributions to mathematics, multiscale and otherwise. The United States is perceived to be on the cutting edge of this research. Focusing on multiscale mathematics was a DOE pioneering achievement. The National Science Foundation now has a call out on the theme of multiscale mathematics. ASCR led the field in this effort.

Action: There being no public comment on this topic, a vote was called on the Subcommittee's recommendation. Torczon moved to accept the recommendation with comments. Bell seconded. The vote was unanimously in favor of the motion.

The meeting was adjourned at 11:53 a.m.

Respectfully submitted,
Frederick M. O'Hara, Jr.
Recording Secretary
Nov. 14, 2006

Corrected,
Ellen Stechel
Nov. 17, 2006