Committee of Visitors Report

Advanced Scientific Computing Research
May 2010

Date of COV: May 12-13, 2010
Program: Applied Mathematics
Fiscal Years Being Reviewed: FY07, FY08, FY09
Office: Advanced Scientific Computing Research

Committee Membership:
Andrea Bertozzi, University of California, Los Angeles
Michael Heath, University of Illinois, Urbana-Champaign
Leland Jameson, National Science Foundation
Timothy Kelley, North Carolina State University
Daniel Meiron, California Institute of Technology
Linda Petzold, COV Chair, University of California, Santa Barbara

1. Executive Summary

The Committee of Visitors (COV) for the Office of Advanced Scientific Computing Research (ASCR) program in Applied Mathematics met May 12-13, 2010 at the DOE facility in Germantown, MD.

The COV would like to thank the program officers and ASCR staff who gave of their time and knowledge to help the committee in its deliberations.

Findings and Recommendations:

Based on presentations by, and interviews with program officers and management, as well as examination of project folders in the Applied Mathematics Research program, the COV considers the program to be very effective and well-managed.

Efficacy and quality of the processes used to solicit, review, recommend and document application and proposal actions:

> **Finding:** The solicitation and review processes appear to be effective and fairly administered. The program is to be commended for their work in streamlining the proposal review process. The documentation seems to be done very well. Delays in processing approved grants, which are outside of the control of the Applied Mathematics program office, affect the PIs ability to recruit students and postdocs, and also affect tenure decisions for junior faculty.
>
> **Recommendation:** The committee recommends that further consideration be given to improving the level of outreach as regards to new funding opportunities. The COV is aware that the program usually has a very small window to accept proposals and that this is caused by rules concerning new starts during Continuing Resolutions, government fiscal years, etc. We would like to see the DOE explore a more flexible approach so that the proposal acceptance window could be broadened and thereby enhance the program's ability to attract proposals from a broader cross section of the scientific community. Proposal project descriptions should be limited to 15 pages. The merit review criteria for large multi-investigator proposals should include an evaluation that ensures that the elements of the proposed research are appropriately integrated, coordinated and synergistic, as is the case with other DOE activities such as SciDAC and the EFRCs. Actions should be taken to accelerate the processing of approved grants.

Efficacy and quality of the processes used to monitor active awards, projects and programs:

Finding: The Applied Mathematics research program managers use generally effective mechanisms, including site visits, PI meetings and progress reports, to monitor ongoing projects and collect information about major awards and accomplishments. Overall these mechanisms are effective and maintain the high quality of the research.

Recommendation: Explicit guidelines should be instituted for progress reports, including length and a clear description of the information that should be in the report. For example, all PIs should list publications, presentations, awards, and patents attributable to the project. The metrics for impact (awards, impact on scientific community (not only on mathematics), DOE impact, publications, presentations, etc.) should also be clearly stated and explained.

Within the boundaries defined by the DOE mission and available funding, comment on how the award process has affected the breadth and depth of portfolio elements:

Finding: The committee finds the portfolio to be exceptionally strong with regards to both depth and breadth. The balance of awards with respect to innovation, risk and interdisciplinary research appears to be appropriate. The committee was very impressed with the long-term perspective of the DOE applied mathematics program and its simultaneous agility at funding new program areas.

Recommendation: The committee is very impressed and has nothing to recommend in this area.

Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected the national and international standing of the program with regard to other applied mathematics research programs that are also focused on the demands of high performance scientific computing and analysis of petascale datasets.

Finding: The DOE Applied Mathematics program has been, and continues to be, of extremely high quality and standing, both nationally and internationally. A great strength of the program is the willingness it has demonstrated to invest in projects with a longer-term perspective than is possible at most U.S. agencies, enabling the support of breakthrough research and ensuring its success and eventual adoption.

Recommendation: The committee is very impressed. We recommend to continue along the lines noted above.

2. Introduction

A charge letter from the Director of the Office of Science to the Chair of ASCAC, dated October 30, 2009, established the Applied Mathematics Committee of Visitors (COV). The Associate Director of ASCR in consultation with the ASCAC Chair selected the COV chair, announced the formation of the COV at the November 3-4, 2010 ASCAC meeting, and assembled the COV members thereafter. The list of members of the COV is provided in Attachment I, and the charge letter is provided in Attachment II. The COV conducted telephone and email exchanges with the Applied Mathematics program directors, and had a site visit on May 12-13, 2010 (see Attachment III).

This report presents the findings and recommendations of the COV. The on-site visit at the DOE Germantown location was held on Wednesday, May 12 and Thursday, May 13, 2010. COV Chair Linda Petzold discussed the charge to the committee, and Christine Chalk discussed the DOE conflict of interest policy. Sandy Landsberg described the Applied Mathematics program goals and accomplishments along with the approach used to evaluate proposals. After the program summary, the COV and the ASCR Applied Mathematics office managers reviewed program folders that included documentation for both DOE national laboratory and university-led proposals. The COV met in executive session to discuss preliminary findings, and requested further information. On the second day of the review, the requested additional information was presented and discussed by the program managers. At the end of the second day, a summary of the COV's findings and recommendations was discussed with Sandy Landsberg. The final report was prepared using email exchanged between COV members. The COV is very grateful for the active and helpful engagement of the ASCR program managers throughout the review process, including the COV website where many program materials were made easily available before, during and after the meeting.

The specific charge to the COV included the following two major program elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
    a. Solicit, review, recommend, and document proposal actions, and
    b. Monitor active projects and programs.
2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
    a. The breadth and depth of portfolio elements, and
    b. The national and international standing of the program with regard to other applied mathematics research programs that are also focused on the demands of high performance scientific computing and analysis of petascale datasets.

3. Efficacy and Quality of the Program's Processes

The COV found the Applied Mathematics program to be very effective and well-managed. The program officers are dedicated and competent public servants who have considerable knowledge of their portfolios and of the Applied Mathematics community. The program has been, and continues to be, of extremely high quality and standing, both nationally and internationally. The committee was very impressed with the long-term perspective of the program and its simultaneous agility at funding new program areas. The balance of awards, between both laboratory and university investigators, and between continuing and new awards, appears to be quite appropriate. There were 49 laboratory projects vs. 49 university projects, where 70% of the funding went to DOE national laboratories and 30% to universities. With respect to new awards, approximately 80% of awards (both laboratory and university) were renewed, but sometimes PIs change topics. In addition, of the significant growth of the program since FY07 (from $30million to $45 million), almost all has gone to new awards.

Charge Ia: Assess the efficacy and quality of the processes used to solicit, review, recommend and document proposal actions.

The Applied Mathematics program is largely very effective in its processes to solicit, review, recommend and document proposal actions. Solicitation is done in the traditional way such as announcements on the program web pages and use of federal program web sites such as Grants.gov. Laboratories utilize a point of contact (POC) with the program managers, so here the communication is more direct. The review of proposals is a rigorous process involving panel or mail-in reviews depending on the nature of the proposal or program. Typically three reviews are used to evaluate a proposal with the final recommendation resting with the program manager and their superiors. A document control system (PeerNet) is used initially to track submission of the reviews as well as to ensure the proper levels of confidentiality. Later, the proposal, all reviews and documentation detailing the decision process are collected on a protected document repository that is now seeing increasing use by the Office of Science. The committee was quite impressed with the rigor applied to the proposal review and decision process. It was noted that this represents a significant improvement from previous COV reviews where it occasionally proved difficult to retrieve specific documents. The program managers are to be commended for these developments.

We recommend that project descriptions be limited to 15 pages. The merit review criteria for large multi-investigator proposals, including unsolicited proposals, should include an evaluation that ensures that the elements of the proposed research are appropriately integrated, coordinated and synergistic, as is the case with other DOE activities such as SciDAC and the EFRCs.

It was noted that there may be further opportunities for the program to improve the solicitation and submission process. First, there is an impression (based on anecdotal input) that announcements of future DOE programs are not disseminated as broadly as might be desirable. This is apparently not a problem for the DOE laboratories, which typically have points of contact (POCs) who are in direct communication with ASCR

Program managers. But in the academic sphere it would be useful to explore approaches to more widely disseminate the announcements of upcoming programs. For example, this might be achieved through the use of mass e-mailings to interested members of the academic community. Another approach might be to use subscription services such as RSS so that potential investigators are notified of new programs in as timely a manner as possible. It was also noted that once a potential PI is aware of a program it is sometimes the case that the lead time for response to the solicitation can be fairly short. It was explained to the committee that this is sometimes inevitable because it is not known whether a program will be funded until the DOE budget is approved and this sometimes results in tight deadlines for response. The problem with this approach is that it may prove impossible for a highly qualified PI to respond. The committee feels that this is an important issue and that potential remedies should be discussed with senior DOE management.

The committee finds that delays in processing approved grants, which are outside of the control of the Applied Mathematics program office, affect the PIs ability to recruit students and postdocs, and also affect tenure decisions for junior faculty.

Finding: The solicitation and review processes appear to be effective and fairly administered. The program is to be commended for their work in streamlining the proposal review process. The documentation seems to be done very well. Delays in processing approved grants, which are outside of the control of the Applied Mathematics program office, affect the PIs ability to recruit students and postdocs, and also affect tenure decisions for junior faculty.

Recommendation: The committee recommends that further consideration be given to improving the level of outreach as regards to new funding opportunities. The COV is aware that the program usually has a very small window to accept proposals and that this is caused by rules concerning new starts during Continuing Resolutions, government fiscal years, etc. We would like to see the DOE explore a more flexible approach so that the proposal acceptance window could be broadened and thereby enhance the program's ability to attract proposals from a broader cross section of the scientific community.. Proposal project descriptions should be limited to 15 pages. The merit review criteria for large multi-investigator proposals should include an evaluation that ensures that the elements of the proposed research are appropriately integrated, coordinated and synergistic, as is the case with other DOE activities such as SciDAC and the EFRCs. Actions should be taken to accelerate the processing of approved grants.

Charge 1b: Assess the efficacy and quality of the processes used to monitor active awards, projects and programs

Finding: The Applied Mathematics research program managers use generally effective mechanisms, including site visits, PI meetings and progress reports, to monitor ongoing projects and collect information about major awards and

accomplishments. Overall these mechanisms are effective and maintain the high quality of the research.

Recommendation: Explicit guidelines should be instituted for progress reports, including length and a clear description of the information that should be in the report. For example, all PIs should list publications, presentations, awards, and patents attributable to the project. The metrics for impact (awards, impact on scientific community (not only on mathematics), DOE impact, publications, presentations, etc.) should also be clearly stated and explained.

A report template would make it easier for PIs to prepare the progress reports and easier for DOE to evaluate them. Other funding agencies such as the NSF (Fastlane) and ARO do this.

The committed feels that the effort the DOE invests in monitoring should be commensurate with the size of the grant. This seems to be the de facto policy, but is not explicit.

4. Effect of the Award Process on Portfolios

Charge 2a: Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected the breadth and depth of portfolio elements.

The new target initiatives have considerable breadth as well as depth. In terms of breadth, the target solicitations identify novel funding areas for the DOE – the last few fiscal years' topics of Multiscale Mathematics and Optimization of Complex Systems, Mathematics for Analysis of Petascale Data, and Mathematics for Complex, Distributed, Interconnected Systems have identified new areas of high priority for research in applied mathematics, that also embrace the core DOE missions. They also branch out into areas that are related to but not the same focus as prior DOE areas of funding in applied mathematics – one example being Analysis of Petascale Data – in which a number of the funded projects are not looking necessarily at data from numerical simulations but rather many modes of data generated from sensors, field studies, and other diverse DOE application areas. The committee was impressed with the depth and impact of several DOE-funded projects, for example adaptive mesh refinement, level set methods, highly scalable Maxwell solver for electromagnetics problems, PETSC, petascale algorithms for transport simulation, and mimetic methods for PDEs.

The committee considered the balance of awards with respect to innovation, risk, and interdisciplinary research. The Applied Mathematics funding portfolio appears to be well-balanced. The program has definitely evolved with respect to new science thrusts, and has

been very proactive in anticipating the implications for applied mathematics research areas of the evolution of DOE's overall portfolio.

The committee examined the evolution of the portfolio with respect to new investigators and new science thrusts. The balance appears to be quite appropriate.

The committee was very impressed with the long-term perspective of the DOE applied mathematics program and its simultaneous agility at funding new program areas.

Finding: The committee finds the portfolio to be exceptionally strong with regards to both depth and breadth. The balance of awards with respect to innovation, risk and interdisciplinary research appears to be appropriate. The committee was very impressed with the long-term perspective of the DOE applied mathematics program and its simultaneous agility at funding new program areas.

Recommendation: The committee is very impressed and has nothing to recommend in this area.

Charge 2b: Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected the national and international standing of the program with regard to other applied mathematics research programs that are also focused on the demands of high performance scientific computing and analysis of petascale datasets.

The DOE Applied Mathematics program has been, and continues to be, of extremely high quality and standing, both nationally and internationally. As one quantitative measure, the program has funded a substantial fraction of the members of the National Academy of Engineering in computational mathematics and the members of the National Academy of Science in applied mathematics. In most of these instances, DOE has funded these Academy members since early in their careers, long before they reached their current distinguished status. Similarly impressive statistics could be cited for other measures of the quality of its investigators, such as Fellows of relevant professional societies and editorships of top quality journals.

We know of no other program whose scope is directly comparable with that of the DOE Applied Mathematics program. The NSF Applied Mathematics and Computational Mathematics programs fund some research that is complementary to the focus of the DOE Applied Mathematics program. The DOE Applied Mathematics program is highly competitive in terms of quality and productivity. Moreover, the DOE program benefits from greater integration of applied and computational mathematics with high performance scientific computing.

The DOE Applied Mathematics program has also been highly successful in pushing the frontiers in new areas, such as uncertainty quantification and petascale data analysis, in which the program has already initiated fundamental, broad-based programs with multiple funded projects already underway, while other agencies are still studying the possibility of

initiating new programs in these areas or are sponsoring only limited projects that are narrowly focused on specific programmatic agency needs. For example, the Applied Mathematics program on petascale data analysis is distinguished by its breadth and by its emphasis on unstructured data sets where little is known in advance about what information they may yield. It is too soon to tell how some of these newer projects will turn out, but these Applied Mathematics programs have a clear lead that could well result in a dominant position in these emerging areas.

The program has an impressive track record in establishing fruitful new areas of research and moving into them nimbly and quickly. The teamwork and coordination between DOE Applied Mathematics and its sister programs within ASCR has also contributed to the agility just noted.

A great strength of the DOE Applied Mathematics program is the willingness it has demonstrated to invest in projects with a longer-term perspective than is possible at most U.S. agencies, enabling the support of breakthrough research and ensuring its success and eventual adoption. Illustrative examples include adaptive mesh refinement for PDEs, the PETSc toolkit for high performance scientific computing, and level set methods for tracking moving interfaces.

Finding: The DOE Applied Mathematics program has been, and continues to be, of extremely high quality and standing, both nationally and internationally. A great strength of the program is the willingness it has demonstrated to invest in projects with a longer-term perspective than is possible at most U.S. agencies, enabling the support of breakthrough research and ensuring its success and eventual adoption.

Recommendation: The committee is very impressed. We recommend to continue along the lines noted above.

Attachment I

ASCR Applied Mathematics Committee of Visitors

Andrea Bertozzi
University of California, Los Angeles

Michael Heath
University of Illinois, Urbana-Champaign

Leland Jameson
National Science Foundation

Timothy Kelley
North Carolina State University

Daniel Meiron
California Institute of Technology

Linda Petzold, COV Chair
University of California, Santa Barbara

Attachment II

Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 30, 2009

Dr. Roscoe Giles, ASCAC Chair
Department of Electrical and Computer
Engineering
Boston University
8 St. Mary's Street
Boston, Massachusetts 02215

Dear Dr. Giles:

Thank you for the excellent Committee of Visitors (COV) review of the Computer Science program. The Office of Advanced Scientific Computing Research (ASCR) has already undertaken changes to respond to the recommendations of the COV and improve the management of this important program. The full program response and action plan is posted on the Advanced Scientific Computing Advisory Committee (ASCAC) website (http://www.sc.doe.gov/ascr/ASCAC/Reports.html).

To help the research communities utilize the capabilities of current and future supercomputers, ASCR also supports a basic research program in Applied Mathematics. To ensure the integrity of this research program, I am asking the (ASCAC) to assemble a COV to review the management processes for the Applied Mathematics elements of the ASCR program. A report will be expected at the August 2010 ASCAC meeting.

The COV should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. The Committee should assess the operations of the Applied Mathematics programs during the fiscal years 2007, 2008, and 2009. The panel may examine any files from this period for both DOE laboratory projects and university projects. The Committee will be provided with background material on the program prior to the meeting.

I would like the Committee to consider and provide evaluation of the following two major program elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
   (a) solicit, review, recommend, and document proposal actions, and
   (b) monitor active projects and programs.

2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
   (a) the breadth and depth of portfolio elements, and
   (b) the national and international standing of the program with regard to other applied mathematics research programs that are also focused on the demands of high performance scientific computing and analysis of petascale datasets.

If you or the COV Chair have any questions, please contact Christine Chalk, the Designated Federal Official for ASCAC at 301-903-5152 or by e-mail at christine.chalk@science.doe.gov.

I appreciate ASCAC's willingness to undertake this important activity.

Sincerely,

W. F. Brinkman
Director, Office of Science

Attachment III

Wednesday, May 12, 2010

8:30-9:00	Introductions and continental breakfast
9:00-9:15	Discussion of Charge to the COV, Linda Petzold, COV Chair
9:15-10:45	Overview of Applied Math and Committee Questions, Sandy Landsberg
10:45-11:00	Break
11:00-12:30	Question and answer session, COV members and ASCR staff Organization of COV documents, Sandy Landsberg
12:30-1:00	Lunch (pick up from Cafeteria or Rick's stand)
1:00-2:30	COV working session: Discussion of Applied Math strategic plan and direction
2:30-2:45	Break
2:45-5:00	COV working session: Discussion of Applied Math process for solicitation development, proposal review and selection, and award monitoring
5:00-6:30	COV working session: Discussion of Applied Math portfolio and standing with regard to similar programs
6:30	Adjourn until dinner
7:00	Committee Dinner

Thursday, May 13, 2010

8:30-9:00	Opening remarks and continental breakfast
9:00-9:30	Question and answer session, COV members and ASCR staff
9:30-10:30	COV working session: Report planning and outline development
10:30-10:45	Break
10:45-12:30	COV closing discussion and review of writing assignments and deadlines
12:30	Adjourn