Report
To
Basic Energy Sciences Advisory Committee

Committee of Visitors
For
Basic Energy Sciences Scientific User Facilities Division

I. Introduction

The Office of Science has instituted Committees of Visitors (COV) for all of its major program areas to evaluate the efficiency, program quality, and administration. Previous BES COVs have reviewed the Materials Science and Chemical Sciences Programs and have contributed to the process of BES program management. These reviews were patterned on the Committees of Visitors established for the NSF, which has a long, established history of such reviews. The BES reviews had to deal with the complexities of mixed individual investigator grants, laboratory Field Work Proposals, and facility use.

The present review, which deals with the newly established Scientific User Facilities Division, has required further extension of the ideas and methods of review. The individual budgets of facilities are large by comparison with typical program grants, and peer review is of necessity somewhat different. In addition the Division is a new organization, which is still in the process of defining its methods and procedures. This makes this review more difficult, but also possibly even more influential in establishing the policies and procedures for the future.

Before beginning our report we want to thank the BES staff, both from the Scientific User Facilities Division and from the program Divisions, for their generosity with their time and for their full and open discussions with us. We also want especially to thank Pat Dehmer for her availability for our discussions, and for the total support that she showed for the COV process in particular and for response to oversight in general.

II. The Charge

The charge to the COV was formulated by the Director of BASIC ENERGY SCIENCES, Patricia Dehmer as follows:

> "1. For the scientific user facilities, assess the efficacy and quality of the processes used to:
>
> (a) solicit, review, recommend, and document actions leading to upgrade or construction of facilities or to special research activities related to facilities such as detector development or accelerator physics, and
> (b) monitor operating facilities.
>
> 2. Comment on how this review process has affected the national and international standing of the individual facilities and the collection of facilities operated by BES.
>
> The panel will assess actions beginning with the 1997 (Birgenau/Shen) review of the BES light sources. This scope of activities under review will include BESAC reviews of all of the major facilities and subsequent BES reviews of the nanoscale science research centers, the light sources, and the neutron sources during this period. The panel will be able to examine all of the BESAC reports and all of the BES files during this period.

The meeting will be scheduled for March 9, 2004, with an evening reception tentatively scheduled for Monday, March 8, 2004."

The Meeting was held at DOE, Germantown on March 9-10, 2004, with a working dinner preceding the meeting on March 8. The COV, with the concurrence of Dr. Dehmer, interpreted the charge broadly, and addressed a range of issues facing the Division.

III. The Committee Composition

The Committee comprised 9 people with a broad range of experience as facility users, facility directors, research managers and reviewers. Many of the Committee members have previously served on BESAC, and two served on earlier COVs. The members of the Committee were:

Dr. Ian Anderson, Oak Ridge National Laboratory
Dr. Nora Berrah, Western Michigan University
Dr. Martin Blume, The American Physical Society
Dr. Miles Klein, University of Illinois UC
Dr. Richard Osgood, Columbia University
Dr. Thomas Russell, University of Massachussetts
Dr. Sunil Sinha, University of California, San Diego
Dr. J. Michael Rowe, NIST (Chair)
Dr. Julia Phillips, Sandia National Laboratories

During the review, members of the COV recused themselves from any discussions in which they could have a real or perceived conflict of interest.

III. The Review Process

This COV review is distinguished from the earlier two reviews by the following points:

- The Scientific User Facilities Division is new within the BASIC ENERGY SCIENCES structure, so that processes, policies and procedures are still being developed.

- Each facility is in itself a large entity, with a total budget equivalent to many individual PI grants.

- The peer review process is of necessity different for a facility and a PI grant. In fact, the facility reviews have been done in two different modes:
    - As a full BESAC subpanel review (e.g. Birgeneau/Shen review of synchrotron radiation sources)
    - As independent peer reviews by groups of reviewers who submit separate reviews (e.g. reviews of APS, HFIR)

As a result of these distinctive features, the COV proceeded in a somewhat different mode than the earlier two COV reviews. The Committee heard presentations by Pat Dehmer and Pedro Montano, and spent two hours probing the COV process, the rationale for this new division, and the audience for the COV report. The members then divided themselves into three groups to

look at review histories for Synchrotron Radiation, Neutron Source and the new NanoScience Centers. During the course of the meeting, each of the members looked at representative folders from each of the groups, in addition to their primary assignment. The COV also spent several hours in executive session, exploring the over-riding issues that faced the Division and BES.

V. Discussion of Review

1. The COV Process for the review

The committee was generally happy with the overall design of the Review. We found it essential to have access to the BESAC reports and BES files for the covered period (1997 to the present), to have ample time for discussions with BES staff, and to have time for closed discussions.
The charge to our COV was adequate. After due discussions with the BES leadership, we chose to expand on those issues within the charge that we thought were most timely and important.

Drs. Dehmer and Montano presented brief summaries of the history of Reviews carried out by BES of their Facilities and of the Nanoscale Science Research Centers. These were helpful, but for future COV reviews of the Facilities Division we ask that the history presentation contain Timelines of the Review history for each Facility or Center. Each Timeline should take the form:

> Review–>Recommendations–>Results (including the written response to the COV/BESAC)[–>Re-Review and its Results, when necessary]

In the front of the jacket for the most recent review for each facility, it would be useful to have a brief document that records the review history for the facility. This would include the dates of the reviews, review findings, laboratory response to the findings, and significant actions taken by BES and/or the laboratory in response to those findings, e.g., re-reviews, changes in funding, personnel, facility direction, etc. Cross-references to the full jacket for previous reviews would also be useful.

2. Documentation of Facility Reviews

There are several elements that should be contained in the report and file of *every* BES facility review; we note that in many cases the reviews did include these elements but their inclusion was not uniform. These are enumerated below:

- There should be an Executive Summary that accurately reflects the substance and tone of the entire document. Major recommendations and conclusions, both critical and complimentary, should be highlighted in proportion to their appearance in the report. Some readers might never get beyond the Summary and they should not carry away an impression that would change substantially should they read the report in its entirety. The report itself should be succinct and clearly laid out.

- BES should prepare and distribute letter responses to the reviews. The distribution should include the management of the facility being reviewed as well as the upper management of the host institution of the facility. Action items should be identified and a further response requested from the facility.

- If possible, copies of the BES and facility responses should be distributed to the review committee. The purpose of this distribution is to assure members of the committee that their report has been interpreted properly and that their most significant points have been taken into account. (Several members of the COV were seeing for the first time at this meeting the results of reviews in which they had participated in the past, and observed that it would have been valuable to have seen them much earlier.) If it is not possible to send the full documentation, then a letter to the committee stating in general terms the facts of the responses and outcomes would give a sense of action to the committee.

- In the case of facilities reviews that are not carried out by a BESAC subcommittee, the individual reviews are generally sent verbatim to the facility. The reviewers should be informed that this is the case, and that in the future a Committee of Visitors will have access to the individual reports.

- A re-review might be necessary if significant findings call for action by the facility. This should be done on a timely basis, considerably sooner than called for by the standard schedule. This could be a progress review, with fewer reviewers, but should have real teeth.

3. Users of Facilities

The success of the Scientific Facilities Division depends critically on satisfying the needs of the "user" community. As a result the committee felt strongly that it was crucial to have a clear and current definition of who exactly is a user. For example, our understanding is that the current DOE definition of a user includes the requirement that this person actually be present when an experiment is undertaken. This requirement appears to be at odds with the fact that many actual "uses" of facilities are now done remotely and that this trend is increasing. Protein crystallography is a good case in point. Within the nanocenters, this remote usage may be pervasive with certain types of instruments such as the most expensive e-beam writers. Having an accurate definition of a user will lead to more accurate counting of the number of people taking advantage of the facility and most probably this number will increase.

4. Metrics

Evaluation of the success of facilities is now being done on the basis of quantifiable metrics. The Committee was strongly in favor of this approach since it allows a rational basis for comparison of the performance and the utilization of each of the DOE facilities. An excellent example of a successful implementation of this approach is the series of questions on publications, beamline performance for synchrotrons, etc. These metrics should be periodically examined and input from the facility directors taken into consideration. At present some of the

metrics appear to need revision. For example, while a list of numbers from the citation index of papers published by users is very useful, the use of this list for papers published in the last 1-2 years seems questionable or even meaningless. A second example is the issue of cost per given quantity of, e.g. papers or beamlines. The intent of these metrics is excellent, however, there is apparently concern about whether there is a uniform and well established understanding of cost. While many metrics will be useful and appropriate for all user facilities, the differences between the various types of facilities make it likely that there will be important differences in the full set of metrics appropriate for the very large facilities (e.g., synchrotron radiation and neutron sources) and the smaller ones (e.g. nanoscience centers and, likely in the future, electron beam facilities). Each set of metrics must be designed to drive the desired behavior for a particular facility.

5. Facility Review Process

The committee, based on surveys of the documentation available, felt that the facility reviews conducted by both BESAC and BES were carried out in an equitable and fair manner and were accepted as such by the facilities themselves. There is, however, considerable unease about the use of individual rather than consensus reports, which may be partially alleviated by the COV reviews and by ensuring adequate opportunities for facility responses. The reviews of the facilities carried out by BES are programmed in a regular fashion, typically on a 3-year cycle. In many cases these reviews have had salutary effects on the performance of the facilities.

The COV is concerned that limited travel funds are restricting participation of scientific program managers in facility reviews. In our view, close coordination with the science programs is essential to success. In fact, the scientific program managers are essential stakeholders in the scientific user facilities.

The BES review reports are not documented or presented to the facilities in the form of a consensus arrived at by the whole committee. BES should carefully consider whether this process may be perceived as open to criticism, and should actively seek ways to allay any possible appearance of bias that could arise. The COV process itself plays a major role in forestalling such criticisms, and more explicit instructions and comments to reviewers and reviewees, including summary reports of actions taken (within the boundaries of necessary confidentiality) could also help. From our reviews and from comments made by facility directors, we are absolutely confident in the integrity of the reviews to date.

We would like to offer the following suggestions to improve the review process:

> BES should think critically about the Metrics that it requires from the facilities in preparation for the review process, since a large amount of effort may be required in the production of a parameter that may not provide a useful evaluation of the performance of a facility. A survey of users of the facility should be required, to be carried out by the users committees, which should contain at least some prescribed items, and a summary of the users' responses should be available well before the time of the review.

The reviews should be structured on a less tight schedule, so that there is considerably more time for executive discussions within the review committee, even at the expense of time for formal scientific presentations. More emphasis should be given to the strategic plans of the facility management, and to the interaction of the facilities with the overall laboratory strategic plans and goals.

Time should be set aside during the review for the review committee members to have the opportunity for informal interactions with users, and facility staff, in particular junior staff.

If the review report indicates serious deficiencies in the functioning of a facility, we would suggest that in addition to requiring that the facility provide a formal, written response to the criticisms and required action items, the facility should be re-reviewed within a short time.

In addition to allocating more time for Executive Discussions during the review, the committee felt that specific time should be set aside during a review for presentation *and discussion* of individual-laboratory-related issues. Typically, at present, a presentation is given on these issues but the discussion time for that area is rather limited.

6. Nanoscale Science Research Centers

The five nanoscale science research centers (NSRC), currently being built simultaneously, represent the newest class of User Facilities funded by BES. As such, there is a unique opportunity to encourage (require) cooperation and collaboration amongst the centers, especially since they plan to have similar as well as complementary instruments. We thus strongly recommend that BES encourage the centers to establish processes amongst themselves in order to cooperate and collaborate scientifically and to formalize a process that will allow users to utilize more than one of the five facilities if needed for their research.

We also strongly recommend *broad users'* input at all stages of the construction of the five centers, since they are designated as national user facilities. The involvement of the users should be sought while the facilities are designed, built, evolve and mature, since this input can contribute significant aspects that may not be relevant after the facilities are built. We also recommend that satisfaction polls/surveys of the nanoscale research community be conducted at workshops and users meetings of all five centers at least once a year to provide timely feedback to each facility as well as to BES reviews of the facilities.

Key elements in locating NSRCs at specific national laboratories were the well-established expertise at the laboratories in scientific areas relevant to nanoscience and the existence of national x-ray and neutron sources and electron microscopy facilities that are critical for the characterization of nanostructured materials. While efforts to organize the centers are well underway, it was evident from our review that formal relationships between existing programs and facilities with the NSRCs were not in place. At this stage in the development of the NSRCs, it is appropriate to formalize the responsibilities and commitments of the laboratories to the

centers, and *vice versa*, memoranda of understanding need to be set in place. These MOU's should clearly define the access of the users of the NSRCs to facilities at the laboratories, including instrumentation and laboratory space, and the access of the host laboratories to the facilities within the NSRCs. Formalizing these interactions is essential to distinguish the program associated with the NSRCs from the core programs at the laboratories.

The NSRC program has, from the beginning, been designed to develop a national resource, establishing a user program to provide the research community immediate access to emerging capabilities in the area of nanoscience. As a national resource, this program requires co-ordination between the laboratories, so as to optimize the use of the facilities and maximize the output of scientific and technological advances. Each center is located at a laboratory with a distinct expertise and unique characterization capabilities. Efforts need to be made to institute an integrated national system that is transparent to the user and independent of any particular NSRC. An integrated system will also enhance the scientific and technological output and serve to make the centers a national, as opposed to a local, resource.

An additional concern of the COV was the manner in which the centers will integrate into the core programs at the DOE and how the research endeavors at the NSRCs can best serve the mission of the DOE. This requires a scrutiny of the management of the centers, the integration of the NSRCs with the laboratories, and an alignment of the overall objective and mission of the centers with the core programs. This would serve to optimize the use of limited funds available for research and instrumentation, facilitate advances in the core programs, and formulate a broad user base for the NSRCs. Research efforts at the centers span all divisions in BES and coordination with and integration into the core programs will leverage available resources.

VI. Conclusions

The COV has concluded that the newly constituted Scientific User Facilities Division is well launched, and is already operating well. The facility reviews are considered fair by the facilities and by the COV, and have had significant impact on several facilities (although many of the reviews occurred prior to the formation of the Division, we have considered them in this review). Throughout the body of this report, we have made recommendations for improvements and changes in the review process, but, on the whole, we are satisfied that the Division is on the right track, and expect further salutary effects from its establishment, both in facility operation and in scientific program management (since facility responsibilities were necessarily monopolizing management bandwidth in the prior arrangement). We urge careful attention to the coordination between the two major science program divisions (Materials Sciences and Engineering and Chemical Sciences, Geosciences and Biosciences) and the Scientific User Facilities Division, and strongly recommend that science program managers attend and participate in all facility reviews.

We strongly support the establishment of the Nanoscale Science Research Centers, and encourage the Division to take a strong hand in exploiting the unique opportunity presented. To this end, we have made recommendations for national planning and cooperation, and for strong user input throughout the entire process.

Committee of Visitors – Scientific User Facilities Division
March 8-10, 2004
Agenda
DOE/Germantown Building
Conference Room: E-401

	Monday, March 8, 2004	
6:30 pm	Dinner This could be Executive Session of the Committee; or with senior members of the Scientific User Facilities Division and BES (Pat and Pedro); or with all staff of the Scientific User Facilities.	Marriott Gaithersburg Washingtonian Private Dining Room
	Tuesday, March 9, 2004	
7:30 am	Shuttle Pickup in Front of Hotel	
8:00 am – 8:30 am	Executive Session Continental Breakfast available to the Committee in Conference Room E-401	
8:30 am – 9:00 am	Welcome and Introduction to BES and the COV process	Pat Dehmer
9:00 am – 9:30 am	Overview of the BES major user facilities and the peer review process	Pedro Montano
9:30 am – 10:00 am	Q&A with staff of the Scientific User Facility Division	COV members and BES staff
10:00 am – 10:15 am	BREAK	
10:15 am – 12:00 pm	Executive Session – Review files and jackets	COV members BES staff on call
12:00 pm – 1:00 pm	LUNCH	
1:00 pm – 4:00 pm	Executive Session – Review files and jackets	COV members BES staff on call
4:00 pm – 5:00 pm	Discussion with BES staff	COV and BES staff
5:00 p.m.	Shuttle to Hotel	
	DINNER	
	Wednesday, March 10, 2004	
7:30 am	Shuttle Pickup in Front of Hotel	
8:00 am – 8:30 am	Executive Session Continental Breakfast available to the Committee in Conference Room E-401	
8:30 am – 12:00 pm	Executive Session – Review files and jackets Draft report and recommendations	COV members BES staff on call
12:00 pm – 1:00 pm	LUNCH	
1:00pm – 2:00pm	Executive Session – Review files and jackets Draft report and recommendations	COV members BES staff on call
2:00pm – 3:00pm	Closeout Session	COV members and BES staff
3:00pm	ADJOURN	

Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 17, 2003

Professor John Hemminger
Department of Chemistry
University of California, Irvine
Irvine, CA 92697

Dear Professor Hemminger:

Thank you very much for agreeing to chair the Basic Energy Sciences Advisory Committee (BESAC). I very much appreciate you taking on this important function for the Office of Science. This year, I would like BESAC to take on two charges:

1. The August 10, 1999, charge to BESAC instituted Committees of Visitors (COV) to assess the program management of major elements of the Basic Energy Sciences (BES) program every three to four years. The first two COV reviews–of the chemical sciences research activities in January 2002 and the materials sciences and engineering research activities in March 2003–resulted in many improvements to the peer review process. These reviews were of great benefit to the BES program managers and to me. I know that you served as a member of the first COV review and the Chair of the second, and I want to thank you for your help in establishing COVs in the Office of Science. I would now ask BESAC to conduct a COV review of the activities within the new Scientific User Facilities Division. A report to BESAC should be planned for the summer or fall 2004 BESAC meeting.

2. Next, I would like BESAC to empanel a subcommittee to consider theory, high-end computing, work-station/cluster computing, and algorithm development as they pertain to the research activities of the BES programs. Although there have been several such studies in the recent past, none were specific to the BES research communities and none sought to comprehensively look at all of these elements simultaneously. The subpanel should have at least one member of the Advanced Scientific Computing Advisory Committee to provide liaison with that group. You should work with the subcommittee chair to refine a charge; however, at a minimum, I would like the study to address the following:

(a) Identify and assess the major opportunities to advance the research supported by the Basic Energy Sciences program through high-end computing (HEC) and through conventional (workstation and cluster) computing. Summarize recent past and projected future scientific impacts of each.

(b) Identify research areas supported by the Basic Energy Sciences program that are now using HEC, are ready to use HEC, or that might benefit from HEC in the near future. Assess the challenges and needs for the use of HEC, e.g., the development of theory, mathematical algorithms, system software, and hardware architectures; the availability of and access to HEC machines and the customization of HEC machines; and the funding requirements.

Please provide a bibliography of recent, relevant studies that you encounter in this study.

Sincerely,

Raymond L. Orbach
Director
Office of Science

Report of COV for BES Scientific User Facilities Division

Presented to BESAC Meeting

August 5, 2004

J. Michael Rowe

Committee Members

- Ian Anderson, ORNL
- Nora Berrah, W. Michigan University
- Martin Blume, APS
- Miles Klein, UIUC
- Richard Osgood, Columbia University
- Thomas Russell, University of Massachusetts
- Sunil Sinha, University of California, San Diego
- Michael Rowe, NIST (Chair)
- Julia Phillips, Sandia National Laboratories

Charge to Committee

- For the scientific user facilities, assess the efficacy and quality of the processes used to:
  - Solicit, review, recommend, and document actions leading to upgrade or construction of facilities or to special research activities related to facilities such as detector development or accelerator physics, and
  - Monitor operating facilities
- Comment on how this review process has affected the national and international standing of the individual facilities and the collection of facilities operated by BES.

The Review Process 1

- This is a new division, still developing policies and procedures, and the scale of projects is quite different from the other two divisions.
- The peer review process is, of necessity, different from PI grant processes
  - Either full BESAC sub-panel review (Birgeneau/Shen)
  - Or independent reviewers submitting individual reports (e.g. APS, HFIR)

Review Process 2

- The charge is quite broad, and with limited time we chose to interpret it broadly and focus on
  - the establishment of the new Division and issues relating to this
  - the review process itself, as applied to synchrotron sources, neutron sources and nano centers

Review Process 3

- Two day meeting in Germantown, 3/9-10
  - Presentations by Pat Dehmer and Pedro Montano
  - Three groups looked at review history for the three major types of facilities, with individual cross-checking of other groups
  - Extensive executive sessions, including discussions with Pat

Review Process 4

- Letters to each BES facility asking for comments (anonymous)
  - All agreed it was fair; all said it helped but…
    - Timing?
    - Differing levels of enthusiasm
  - Definition of metrics
    - Metrics are good, but need careful thought
    - Facilities should be partners in developing metrics
  - Independent reviewers
    - Concern about anecdotes becoming data
    - Appearance of potential for bias
    - Lack of consensus *could* lead to ill-considered statements and recommendations (JMR)

COV Issues

- Complete timelines for each review should be maintained and available for future COVs
  - There were difficulties tracing the process from review to recommendations to results (including facility responses) to re-reviews when necessary
  - Cross-references to earlier reviews would help the COV better grasp the full history

Documentation of Facility Reviews

- Necessary elements (inclusion was not uniform)
  - Executive summary that accurately and succinctly reflects tone and substance
  - Letter responses to reviews to facility and laboratory management
  - Reporting of review outcomes to reviewers
  - Care in informing reviewers for non BESAC reviews of procedures, and that COV will have access in future
  - Re-reviews should be scheduled in cases where the normal schedule is too “leisurely”

Users of Facilities

- Success = happy users and good science
  - User needs are changing, and definitions must follow e.g. mail in samples, remote operation, nano centers
  - Must come to acceptable definition of users, publications, and acknowledgements, when only (small) part of research depends on facility
  - Nano centers will accelerate these trends

Metrics

- The COV approves of the use of well defined metrics in evaluating facilities, with the provisos
  - A countable item may not be a good metric
  - Terms must be clearly defined
  - Metrics for neutron and photon facilities may be different from those for nano centers
- All metrics should be reviewed regularly, in direct consultation with facility managers

Facility Review Process 1

- We conclude that reviews are fair and seen to be so, but there is unease about individual reports
  - May give inordinate weight to minor points
  - Perception by outsiders and facilities
  - COV review and allowance for adequate facility responses help alleviate these concerns

Facility Review Process 2

- Suggestions for improvement
  - Better definition and choice of metrics
  - User surveys should be required (by user groups)
  - The agenda should be controlled to allow more executive discussion
  - Time should always be provided for direct reviewer contact with users and staff
  - When serious deficiencies are identified, we recommend re-review in a short time in addition to written responses
  - Time for discussion of laboratory-wide issues should be included
  - Ensure research program representation at reviews

Nanoscale Science Research Centers

- Recommendations
  - Require inter-center collaboration
  - Closely involve users at the beginning
  - Establish appropriate agreements with other laboratory activities and facilities
  - Coordinate between laboratories to ensure a national, not regional resource
  - Carefully integrate with science programs

General Comments on Division

- New structure is good for all involved
  - Relieves science program managers from details of facility operation
  - Allows research program managers to focus on science
  - Allows facilities to receive proper management attention, commensurate with their budget and impact
  - Reduces scope for budgetary arguments

Then Why Only Now?

- There are actual and potential negatives in separating facilities from science
  - Loss of sense that facilities serve science
  - Decoupling of facility management from research programs
  - Enhanced visibility for good or ill
- We recommend that both research divisions have at least one program manager at every facility review

Conclusions

- The new Scientific User Facilities Division is well launched, building on past facility management
  - COV strongly supports the new structure
  - Facility reviews are working, and we have recommended some changes & improvements
  - We strongly support NSRCs, and recommend national planning and cooperation

Dr. Raymond Orbach
Director
Office of Science
US Department of Energy
1000 Independence Avenue
Washington, DC

Dear Dr. Orbach:

On behalf of the Basic Energy Sciences Advisory Committee (BESAC) I am forwarding to you the report that was requested in an August 1999 charge letter from Dr. Krebs. This report, the Committee of Visitors for Basic Energy Sciences Scientific User Facilities Division, is the result of a Committee of Visitors (COV) that met in March 2004 to address the charge. Dr. J. Michael Rowe of the National Institute of Standards and Technology chaired this committee.

The recommendations of the COV and the contents of this report were unanimously accepted by the members of BESAC at our August 2004 meeting.

I would like to thank you for the opportunity to involve BESAC in this very important review process. The members of the COV believed the new Scientific User Facilities Division was well launched and the facility reviews are working well.

Sincerely,

John Hemminger
Chair
Basic Energy Sciences Advisory Committee

cc: J. Michael Rowe, NIST
Patricia Dehmer
Karen Talamini