REPORT TO THE BIOLOGICAL AND ENVIRONMENTAL RESEARCH ADVISORY COMMITTEE (BERAC)

BY THE COMMITTEE OF VISITORS FOR THE REVIEW OF THE BIOLOGICAL SYSTEMS SCIENCE DIVISION

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I. EXECUTIVE SUMMARY

The Committee of Visitors (COV) reviewed several components of the current Biological Systems Science Division (BSSD) science portfolio that were active during the 2014–2017 period, including the following:

1. Two User Facilities (Joint Genome Institute and Structural Biology Infrastructure program);
2. Four National Laboratory Scientific Focus Area (SFA) programs:
    a. Genomic Sciences: Foundational Genomics;
    b. Genome Sciences: Biofuels;
    c. Radiobiology: Radiochemistry and Instrumentation;
    d. Bioimaging
3. Four University Funding Opportunity Announcements (FOAs):
    a. Genomic Sciences: Systems Biology;
    b. The Plant Feedstock Genomics for Bioenergy Program;
    f. Systems Biology Knowledgebase;
4. Three Bioenergy Research Centers; and
5. Workshops.

The following general comments and recommendations by the COV concern the BSSD and the COV review process. We provide specific comments and recommendations on individual programmatic components in separate sections.

The COV Review Process

The COV commends the BSSD management for making the majority of materials available to the COV members electronically through the PAMs system. The review of materials was efficiently facilitated by this system. We recommend that BSSD complete the process and make all materials available electronically in PAMs for future reviews, and work on improving PAMs so it is easier to navigate and access. The annual reporting system in PAMS was identified by the COV as one of the major successes in process optimization during this reporting period. The OSTI database provides an on-line source of publications from the funded projects, particularly those of National Labs, which are required to use the OSTI system. This requirement should be expanded to all programs funded by the Office of Biological and Environmental Research (BER).

Recommendations

The BSSD has done a commendable job of increasing the number of Program Managers (PMs) working to maintain the broad science portfolio. The PMs should use a wide range of strategies

to gather input into the content of research programs during their development stage. Other COV recommendations are as follows:

1. Particular attention should be paid to promoting research continuity of productive and effective research groups and to stimulating the entry of new researchers into the funding programs.
2. An emphasis on the development of the next generation of scientists should be an ongoing mission of the DOE and BSSD. The COV noted some diffuseness in training mechanisms and plans as articulated in the current SFAs (and FOAs). To strengthen this process, the COV recommends that both academic scientists and those at the National Laboratories be given clear instructions to develop appropriate mentorship plans.
3. Plans should be developed to support the timely upgrades of BSSD-funded synchrotron and neutron experimental stations. Coordination with other government agencies (NIH, NSF, DOD) is strongly encouraged.
4. Better evidence should be presented showing alignment of the programs with the BER long-term goals and the Grand Challenges.
5. The travel funding to support PMs in attending technical meetings is insufficient. The COV recommends increased funding for PM travel to facilitate management of programs and to maintain current knowledge and understanding of technologies being developed worldwide.

II. BIOLOGICAL SYSTEMS SCIENCE DIVISION OVERVIEW AND GENERAL RECOMMENDATIONS

Overview, Findings and Comments

The Committee of Visitors (COV) reviewed the science portfolio of the Biological Systems Science Division (BSSD) of the Office of Biological and Environmental Research (BER), which includes User Facilities, National Laboratory Scientific Focus Areas (SFAs), Bioenergy Research Centers (BRCs), projects funded through Funding Opportunity Announcements (FOAs), and Workshops.

The COV commends the BSSD program for maintaining a balanced portfolio of three different types of funding. The first is the longer-term support provided for facilities such as the Joint Genome Institute (JGI) and Structural Biology Infrastructure program. The second is the stable support provided through the SFA process to both national labs and universities (as subcontractors). The third is the flexible support that is provided via the FOA process, which can be used to respond quickly to arising issues and opportunities. The balance of funding among these three strategies is an important issue for BER-BSSD going forward, especially given the current uncertain funding environment. Thus, we recommend that BSSD PMs carefully consider how to maintain a healthy balance among these three funding mechanisms.

The COV noticed that there is no longer a mechanism for academic institutions to obtain individual grants, except through the FOA process or through collaborations with an SFA. Investigators at the National Laboratories can seek funding from the Laboratory Directed Research and Development program, but more long-term funding is obtained only through the SFA collaborations. The lack of a broader mechanism for submission of research ideas may prevent BER-BSSD from being able to respond quickly to new creative research directions or tools needed to support DOE missions that do not fit into the scope or timing of available FOAs.

The COV commends the BSSD for increasing the number of Program Managers (PMs) within BSSD to 10, with two additional staff members, and for increasing travel support for PMs. During the COV review, the BSSD PMs were immediately responsive to the COV requests for additional and expanded materials. They provided requested documentation when needed and were generous with their time and information. Most material was successfully accessed electronically through the newly adopted PAMs system.

Recommendations

1. Planning for responses to funding reductions should be in place to facilitate the necessary transitions. This is particularly important when dealing with three different funding paradigms that are founded on differential expectations of funding stability. Priorities for maintaining various programs should be transparent.
2. BSSD should consider establishing a mechanism that would permit it to evaluate the occasional meritorious research idea that is not included under active FOAs. The absence of a flexible route for support may affect early-career scientists disproportionately.
3. The Internal Comments section in PAMS should contain a notation on proposals that the PM views as high-risk/high-reward at the time of award. Over time, metadata can be generated to indicate whether or not this initial prediction results in special project outcomes, e.g., high-profile publications and patents. Complete lists of all publications documenting progress of the research efforts under BSSD-funded programs—User Facilities, National Laboratory SFAs, BRCs, and projects funded through FOAs—should be collected by OSTI and made available to the COV prior to the review, and to the public on at least an annual basis. In future reviews, publications should be grouped by program. For example, it would have been helpful to see publications from the synthesis program to more easily judge the productivity of each section of the JGI.
4. As noted in previous COV recommendations, the pre-proposal process should be more selective, such that a smaller number of pre-proposals are advanced to a full submission. This selectivity would reduce the effort of PIs in preparing proposals that will not likely be funded, reduce the workload of the reviewers, and permit more discussion by the review panel concerning which proposals should be funded.

III. BSSD PROGRAM ADMINISTRATION

Overview

On October 5, 2016, Dr. Cherry Murray, Director of the Office of Science, charged the Biological and Environmental Research Advisory Committee (BERAC) with assembling a COV to assess the processes used to create and manage the research portfolio in BER-BSSD. The COV was formed in the summer of 2017 and reviewed four elements of the BSSD science portfolio that were active since the prior COV review:

1. Two User Facilities (JGI and Structural Biology Infrastructure program);
2. Three National Laboratory SFA Programs;
3. The four University FOAs; and
4. Three BRCs.

The BSSD also runs a variety of workshops that engage the research community in defining the most pressing questions and approaches needed to tackle the key questions within BSSD's research portfolio. These were reviewed also.

In response to this charge, a COV was established, consisting of 13 scientists from around the country, with representation from academia (9), National Laboratories (3), and other federal agencies (1). Five of the COV members currently receive DOE funding. One of the COV members served on the prior BSSD COV that met in July 2014. The COV met on 10–12 July, 2017, at the DOE headquarters in Germantown, Maryland. The COV members were assisted and supported, as needed, by the BSSD staff.

To maximize the effectiveness of the analysis, three subcommittees of the COV were formed—each assigned to do an in-depth review of broad and diverse Programs or Projects within the overall BSSD research portfolio. The entire COV evaluated and analyzed the portfolio as a whole, and provided comments and recommendations.

The charge letter asked the COV to assess the following aspects of the operations of BSSD's programs for FY 2014–2016:

- National Laboratories' proposals;
- Academic institutions' grants;
- The quality of the scientific portfolio, including its breadth, depth and national and international standing;
- The BSSD's management and oversight of the JGI and Structural Biology User Facilities;
- The efficacy and quality of the processes used by BSSD for
    - Solicitation, review, recommendation and documentation of applications and proposal actions and
    - Monitoring active awards, projects and programs; and

- How the award process has affected the breadth and depth of the portfolio elements and the national and international standing of the portfolio.

Summary of COV Findings

Overall, the COV was impressed with the quality and management of the solicitation of proposals and the review process. The COV commends the BSSD's role in implementing what we perceive to be a fair and equitable review process that uses the highest standards of the competitive funding community to maintain a vigorous research portfolio. The funded programs have a good balance of risky, solid, and innovative science.

Merit reviews were uniformly conducted with an adequate number of highly qualified reviewers, without obvious conflicts and having appropriate expertise that together provided appropriate panel breadth. In most instances, the time intervals between issuing the SFA/FOA, requiring submissions of pre-proposals and proposals, and announcing decisions were satisfactory, providing investigators ample time for preparation. There was generally good documentation of the proposal review and evaluation process.

Similarly to the previous findings, the COV reports that in a limited number of cases, sparse documentation was found supporting the recommendation for or against funding of submitted proposals. The COV did not feel these awards were inappropriate, just that the documentation for the justification of the award was absent from the files.

IV. REVIEW OF DOE PROGRAMS IN THE BIOLOGICAL SYSTEMS SCIENCE DIVISION

This Division supports a very diverse portfolio of research areas with a rather small number of PMs. In addition to the Division Director, the current staffing includes 10 PMs and one science assistant. Several PMs have exclusive responsibility for several large and essential programs. The COV commends BSSD for hiring three new staff members to serve as the PMs for the Structural Biology Infrastructure program, Microbial Systems Biology, and Computational Bioscience, respectively. An additional biologist needs to be hired to support the Foundational and Analytical Genomic Science Program.

The COV was highly impressed with the SFA and FOA solicitations, reviews, and monitoring activities by the PMs, especially considering the limited funding for travel and for support staff to administer these programs. The COV concludes that the major user programs have been rigorously reviewed, with calls for proposals following a regularized process, leading to a highly productive science program with impactful outcomes. The COV notes, however, that the "Grand Challenge" addressed in each research plan should be evident. This is especially important for the National Laboratory interdisciplinary teams that were established to address more difficult research projects that could not likely be successfully completed in a single-laboratory setting.

In spite of the current challenges, the COV observes that the administration of BSSD programs remains an excellent operation. The BSSD research portfolios are at the cutting edge of a diverse array of research questions that are critically important to national needs.

A. Facilities: Joint Genome Institute

Overview, Findings and Comments

The JGI is a DOE Office of Science User Facility, funded by DOE-BER and operated by Lawrence Berkeley National Laboratory (LBNL). It has long-standing partnerships with Lawrence Livermore National Laboratory (LLNL) and Hudson Alpha, and a more recent one with the National Energy Research Scientific Computing Center (NERSC). The JGI mission is to advance genomics in support of the DOE missions related to bioenergy and the environment. Its main focus as a user facility is to provide the scientific user community with genomics and analysis of plants, microbes, and communities of microbes.

The COV reviewed the following JGI programs:

- Community Science Program (CSP)
- DNA Synthesis Program
- Emerging Technologies Opportunity Program (ETOP)
- Facilities Integrating Collaborations for User Science (FICUS) JGI-Environmental Molecular Sciences Laboratory (EMSL) Collaborative Science Initiative

The JGI model of a user facility is working well and is an efficient way to engage the broader scientific community in the DOE-BER mission, while providing infrastructure and scientific support. For a relatively modest investment by BER, and with an essentially flat budget (~$69M/yr), there has been a 100-fold increase in sequencing output (from ~1.5 to ~150 Tbases) and a 10% growth in users (to ~1,400) in the last three years, i.e. a significant return on the investment to advance the scientific mission. JGI is also a great enabler of scientists who might want to try more risky projects, and of those who have good ideas without sufficient funding for sequencing aspects.

Most of the programs that JGI runs, such as the CSP, have appropriate oversight through a standardized application and review process that includes an external peer-review panel, a technical review, and a final review by DOE-BER program staff. As an example, the CSP issues a call for proposals each year, beginning with a letter of intent that is mainly evaluated for technical feasibility and alignment with the DOE-BER mission. Full proposals are then solicited and evaluated via a peer review process, then ranked by JGI, with final review of the selection by the BER-BSSD PM. In 2017, the CSP received 122 letters of intent; 98 groups were encouraged to submit full applications, and 37 were approved. Given the approximately 30% success rate, it appears that the review process is rigorous. For all approved proposals, a user agreement is

created between the PI and JGI, followed by an immediate scheduling process. The DNA Synthesis Program and the FICUS Initiative follow similar proposal and peer-review processes. The ETOP program seems to be based on a Federal Business Opportunities call, with proposals reviewed internally by JGI.

The COV considers these processes to be entirely adequate. The outcomes from the projects (number and quality of the publications, as discussed in the next section) also suggest that the review process is highly successful.

Interactions between JGI and the BSSD PM are well established and frequent even though the PM is located in Washington, D.C., and JGI is in California. A continuing issue, which was critiqued in the 2014 COV report and has not been adequately addressed, is the severe limitation on DOE-BER internal travel funds, restricting the PM's direct visits to JGI to one trip per year. The COV finds that robust management of such a large program would require, at a minimum, quarterly visits by the PM to enable in-person interactions with the different entities of the organization.

The BSSD PM participates in a weekly conference call, with JGI senior management and partners (the Joint Coordinating Committee) one week and with the JGI Director and Deputy Directors the second week, and with monthly metrics (sequencing, finance) as one of the topics. There are semiannual visits to DOE-BER HQ by the JGI Director, and the BSSD PM attends the yearly user conference at JGI. The BSSD PM is well versed in all of the JGI projects, is actively involved in supporting further developments, and provides excellent stewardship.

JGI is reviewed on a regular basis via a Triennial Review of Science and Operations. Seven issues resulted from the most recent Triennial Review. The process and associated documents were clearly laid out, and the review approach was highly professional and included an extensive review by a large number of external scientists. Written responses were developed by JGI management and presented to and reviewed by BER-BSSD, and all issues were addressed with acceptable solutions. JGI moved on to new planning activities on the basis of the review input. The COV commends the JGI management and BSSD PM for a thorough review, and BER-BSSD for a very proactive, ongoing oversight process in all areas.

The COV appreciates the effort by the BSSD PM to provide easy access for the COV team to the JGI review material electronically via a Google site, as well as well-organized paper document folders.

Breadth and Depth of Portfolio and Standing

The quality of the science that JGI enables was judged by COV mainly in terms of the publications and the high quality of successful collaborations that have been completed or are ongoing.

Community Science Program. This program engages the broader scientific community in the DOE mission through the many sequencing and other new technologies that JGI is currently employing. The conversion of JGI to a National User Facility was initiated in 2004. The program provides state-of-the-art sequencing, with emphasis on plants and microbes. JGI partners with Hudson Alpha to get much of the plant genome sequencing completed in an efficient manner.

CSP currently provides 50% of the sequencing capacity to the general user program as described above, 30% to the BRCs, 10% to the microbial program, and 5% each to technology development and Director's discretionary allocations. In general, the program has broadened, and a shift towards greater scope is underway, as is an increasing focus on data analyses, annotations, and functional assignments.

The COV is very positive about the continued evolution of the CSP program. Overall, the process used for the CSP is efficient and, judging from the quality of the research coming from this program, the COV agrees that this JGI main focus leads to productive and excellent outcomes. JGI has had, on average, ~1200 users per year during the FY 2014–FY 2016 period, who have published 442 papers over this period. With ~1200 users per year, there may be a need to increase capacity, which may be why user surveys showed some concern with the turnaround time. There was evidence that JGI is planning for new instrumentation at the level of $2M/yr, increased automation, and collaboration with industry on less challenging projects.

Each year JGI sponsors a user meeting that is well attended and brings in prominent speakers in different science areas, including plant and microbe science. The meeting also provides JGI the opportunity to showcase and discuss new technologies with users.

DNA Synthesis Program. The DNA Synthesis Program enables users to test hypotheses based on sequence information. This program brings a greater understanding of the function of sequences to the scientific community and DOE. The users make many contributions to the program, including advanced data mining, biological circuit design, sequence assembly, novel microbial strains, and functional characterization. In return, the JGI brings the following to the user community: access to microbe and plant databases, synthetic biology design tools, DNA assembly, cloning and quality control, strains outside of those commercially available for integration, and connectivity to mass spectrometry. The applications to participate in the program have increased from 28 to 42 in a few years and the number of accepted projects is 15–20 per year. The JGI DNA Synthesis Program goes beyond what companies provide. The cost of synthesis at JGI is also very competitive, among the lowest as compared to academic and industry labs. A review of the program was conducted in 2016, providing substantial positive feedback. The review highlighted how this program moves JGI in the direction of functional genomics, which is seen as an important future strategic direction. The program includes some larger collaborative efforts with National Laboratories and with other thematic areas. Calls for proposals are publicized and external reviewers are used to evaluate the proposals. Overall, the way in which projects are chosen appears to be rigorous and contributes to a successful CSP.

Emerging Technologies Opportunity Program. ETOP is an effective way for JGI to tap into expertise outside the Institute to enable better and new science applications. This program accounts for only about 2% of the total budget of JGI, but it is likely to bring new technologies to the Institute and to the science of sequencing and understanding the function derived from sequenced proteins and RNA. The program involves working with some of the top academic labs on special projects and is a new and very exciting feature of the JGI. Projects have led to excellent publications and clearly enhanced capacity.

Facilities Integrating Collaborations for User Science JGI-EMSL Collaborative Science Initiative. The FICUS program is similar to CSP in that scientists are required to submit letters of intent in several different focus areas, after which full proposals are solicited and reviewed. The program is run jointly by JGI and EMSL, building on JGI's sequencing capabilities and EMSL's proteomics capabilities. This brings great synergy to the user community and provides a point of collaboration for both DOE user facilities. Since its initiation in 2014, there have been an average of 10 proposals approved each year in the FICUS program. In recent years, JGI has sponsored a metabolomics or secondary metabolite workshop with many excellent speakers, which should increase the profile of the metabolomics sciences among JGI users. In FY 2017, FICUS was extended to a collaboration between JGI and NERSC, with six proposals approved as a result of this first announcement. FICUS seems to be a highly multidisciplinary and positive program. It forms the foundation for ongoing efforts to expand to a broader interaction and joint programs with additional DOE user facilities.

JGI Interaction with NERSC. The above interaction between JGI and NERSC is viewed very positively by the COV because it provides the Institute with some of the most powerful computing capabilities in the world. JGI spends about 7% of its budget on this computing resource, which seems to be an excellent use of funding. Embedding of JGI staff at NERSC also increases connectivity between the two organizations. The different responsibilities of each organization are clearly delineated in a Memorandum of Understanding, which should further enhance the clear lines of communication between the entities.

Recommendations

1. The partner institution relationships need to be reviewed more rigorously to ensure that JGI is getting the expected level of productivity from its partners. BSSD management could consider including the JGI-NERSC interaction in this review process. The COV recognizes that JGI is providing a critical resource to the BRCs, allocating 30% of the CSP to their projects. However, the COV recommends that the scientific impact of the BRCs' use of the CSP continue to be carefully balanced against the needs of smaller projects and users outside of the BRCs.
2. The COV recommends that if the investment in the ETOP program is significantly increased, enhanced oversight will be needed to ensure that it brings new technologies to JGI and the community, and that appropriate partners are chosen for the projects.
3. The COV recommends that the FICUS program be reviewed.

4. The COV recommends undertaking new strategies to integrate and coordinate JGI and DOE's Systems Biology Knowledgebase (KBase) activities.

B. Facilities: Structural Biology Infrastructure

Overview, Findings and Comments

The Structural Biology Infrastructure program, funded and managed by BER-BSSD, spans broad scientific and technical scopes. The goals of this user facility program are to develop advanced technologies and make them available to the biological research community, and to enable and maximize effective use of DOE's funded National User Facilities. This goal is accomplished in part by providing funding for staff and instrumentation, including beamlines, at the light source and neutron facilities. This BER program jointly funds the national structural biology facilities and infrastructure through arrangements with other agencies, mainly NIH. The ability to coordinate with the NIH is attributable to the outstanding long-term leadership provided by DOE-BER. The COV is pleased to note that succession planning has taken place via the proactive hire of a new PM to oversee this important program. The COV is convinced that the productive interagency coordination with NIH and other agencies will continue, given the new PM's past role at NIH.

The Structural Biology Infrastructure facilities and programs supported by BSSD (~3.4% of the BSSD budget in FY 2016) include those at the following major facilities:

- Advanced Photon Source (APS, at Argonne National Laboratory [ANL]), for macromolecular crystallography;
- National Synchrotron Light Source II (NSLS-II, at Brookhaven National Laboratory [BNL]), for macromolecular crystallography, small-angle X-ray scattering, and imaging;
- Advanced Light Source (ALS, at LBNL), for infrared spectromicroscopy, soft X-ray tomography, macromolecular crystallography, and small-angle X-ray scattering;
- Stanford Synchrotron Radiation Lightsource (SSRL, at SLAC National Accelerator Laboratory), for macromolecular crystallography, small-angle X-ray scattering, X-ray spectroscopy and imaging; and
- High Flux Isotope Reactor/Spallation Neutron Source (HFIR/SNS, at Oak Ridge National Laboratory [ORNL]), for small-angle neutron scattering.

In addition, BSSD co-funds the Protein Data Bank at Rutgers University, one of the most broadly used resources in biology. The BSSD support enables access to National User Facilities by a broad community of biologists, chemists, and environmental scientists.

BER-BSSD and NIH-NIGMS conduct joint proposal reviews using NIH as the lead agency for the synchrotron-based structural biology program facilities at APS, NSLS-II and SSRL, and the X-ray tomography facility at ALS. The program facilities at APS (the Structural Biology Center or SBC), ALS (the small-angle X-ray scattering and infrared spectromicroscopy facilities), and

HFIR/SNS are reviewed solely by BER. On the basis of the documents provided to the COV, the proposal submission, review, agency evaluation and funding decision, and award processes are well documented and performed rigorously. The expertise of the chosen reviewers and the quality of their written reviews were excellent overall. In addition, the PM is well versed in all of the projects. BER has implemented an annual report structure that is applied across all the structural biology user facilities, including feedback provided by the PM. The COV commends this initiative and process. The PM is further actively engaged with the community in processes for developments of structural biology X-ray free electron laser (XFEL) capabilities at the Linac Coherent Light Source (LCLS) at SLAC, and new synchrotron radiation and neutron scattering technologies at the other National User Facilities. The COV has no concerns regarding the performance and quality of the reviews, oversight, or program management.

The PMs have worked with representatives from the respective National User Facility BER programs to create a program of outreach to the BSSD grantees. The goal is to bring together information about BER's structural biology resources on a common web portal (http://www.berstructuralbioportal.org/) with the capacity to inform users about the techniques, previous and current applications, and access processes. This integrated information enables experiments for studying and understanding structural and functional processes of importance to BSSD-funded investigators and centers.

Despite the thorough proposal, review, award, and monitoring processes, built on a peer-review process demonstrating the overall positive impact of the program, there was an overall program budget reduction of ca. 33% in FY 2016, which continued in FY 2017. This has caused a rather drastic reduction in staffing and instrumentation at the facilities, eroding the success of the previous significant investments in scientific capabilities of the BSSD program, as well as curtailing grantee access. The material provided to the COV included no information as to how these decisions were made or the processes undertaken that led to this 33% budget reduction. There was no evidence of consultation with the biology community about the impact of funding reductions on the operation of and access to these facilities.

Breadth and Depth of Portfolio Elements and Standing

The national structural biology facilities have resulted in world-leading transformative science in a wide range of applications. These facilities have enabled the revolutionized understanding of protein structure and function, enzyme mechanisms, and cellular processes, to name a few. The entire field of structure-based drug design has been critically dependent upon the ability to collect high-quality X-ray crystallography data at rapid rates on small crystals. The current and future impact of combining several techniques to probe structure, and thus processes, at various length and time scales cannot be overstated. The emphasis on time-scale experiments is increasing especially rapidly. User demand will continue to be high at synchrotron and neutron facilities and XFEL sources into the foreseeable future. The demand for neutron applications is also expected to grow as beamlines continue operations for structural biology research at the ORNL neutron sources.

The ability to perform experiments via remote access (i.e., while researchers remain at their home institutions) continues to provide high efficiency and productivity and valuable training opportunities while reducing travel costs. The support from highly trained facility staff is critical for continued success. Having access to on-site biochemistry and other wet-lab capabilities at these facilities is also important, as it allows real-time preparation and modification of specimens that enhance the impact and productivity of functional studies. There is also a growing scientific connectivity to the BER Climate and Environmental Sciences Division, in particular with the subsurface biogeochemistry research program. Microbiology is becoming an increasingly important component of this program, and atomic-level structural biology knowledge will be required, using the same toolbox of techniques as in BSSD.

The national and international standing of the structural biology facilities is, at this point, strong. However, with the reduced budget, the ability of this program to support the science of the U.S. biological community in general and the BSSD programs in particular is being eroded and the ability of the grantees to continue or expand their science directions is being curtailed.

This budget reduction comes at a time where the NIH is also restructuring its facility support approach, and together the two partner agencies are shifting the U.S. structural biology landscape in R&D, instrumentation, and facility access and support of the biological community. BER-BSSD, through its Structural Biology Infrastructure program, could take a leadership role nationally through the strategic approach of enhancing its science programs with a focused emphasis on the structural biology facilities.

International investments in structural biology, such as in new facilities, beamlines, and instrument development, are exceedingly high. Elsewhere, there is strong emphasis on integrated structural biology facilities, with technical capabilities spanning a multitude of length and time scales, and with adequate staffing, Examples include the EU/national facilities in Hamburg, Switzerland, South Korea, Brazil, Denmark and Shanghai. The COV is highly concerned that without a concerted effort, the U.S. will fall behind in the development and support of new facilities and infrastructure, which will have a major negative impact on the international competitiveness of the BER Structural Biology Infrastructure program facility as well as its science programs.

Recommendations

1. The DOE-BER-BSSD Structural Biology Infrastructure program is run for the benefit of the entire nation as a part of *Cooperative Stewardship: Managing the Nation's Multidisciplinary User Facilities for Research with Synchrotron Radiation, Neutrons, and High Magnetic Fields.* The COV is concerned about the recent decreases in support and emphatically encourages the continued co-funding of these facilities with NIH and other agencies, and urges the BSSD management to restore the program funding to its

previous level to enable mission-relevant research to be optimally supported at the synchrotron and neutron facilities in the U.S.

2. Another concern of the COV is the lack of substantial funding set aside for capital equipment, which is necessary to keep the U.S. facilities internationally competitive. Although this lack has been partially alleviated by cooperation with other agencies, particularly NIH, it prevents long-term planning of new beamline facilities, major upgrades, and/or the development of new instrumentation tailored to BER's mission needs. In addition, an upgrade of the Structural Biology Center (Sector 19) at the APS will be required in conjunction with the APS Upgrade scheduled for the early 2020s. Investments will be needed at other facilities as well, to enable support of displaced SBC and other APS bioscience users in the estimated 1-year "dark period" currently assumed to occur around 2022.
3. DOE-BER should continue its partnerships with other agencies in supporting the Protein Data Bank. Continued support is essential, given that this data bank influences a wide range of bioenergy research from enzymology to cell biology, nationally and internationally.

C. Laboratory Scientific Focus Area Programs

Overview, Findings and Comments

SFA funding was introduced to all the Laboratories in 2007 to encourage collaborative, interdisciplinary research that would be unlikely to be accomplished in a single-PI academic setting. In general, such projects would be of longer duration and with a larger scope than those identified through FOAs. Topics that are relevant to the BER objectives of clean energy and environment include the following:

- Genomic Sciences: Foundational Science
- Genomic Sciences: Biofuels
- Radiobiology: Radiochemistry and Instrumentation
- Bioimaging

The SFAs were initiated through requests for white papers, followed by requests for full proposals if the research aligned with the BER objectives. Emphasis was placed on the non-competitive nature of the evaluation, which was described as a strictly merit-based review. A panel of expert scientists was asked to evaluate the proposals. The scoring of proposals comprised two parts. The first was a numerical ranking of the proposals (from 10 or 9, Excellent, down to ≤ 4, Poor), with selected descriptors. The second was a recommendation for an action, implemented by the PMs. The following were the possible recommendations:

Accept: PIs should respond to any comments or concerns satisfactorily, as judged by the PMs.

Accept with revisions: Revisions are to be incorporated to the PMs' satisfaction.

Partial acceptance: Only a specific portion of the proposed work is funded. Budget and research plan are to be modified accordingly.
Reject: Proposal was unacceptable on the basis of merit or research area.

Management of the SFAs includes annual reports and Triennial Reviews by an expert scientific panel during a reverse site visit. Additional flexibility in reporting has been used when special cases needed closer supervision. During the FY 2014–FY 2016 period reviewed by the current COV, there were nine SFAs with actions that were within the scope of this review; five were Genomics (Foundational), three were Biofuels (sometimes referenced as Plant/Microbiology), and one was Computational Biology. The Bioimaging effort was initiated during the time of the present COV review.

Foundational Genomics. SFAs in the Genomics area ran the gamut from those with steady progress toward lofty goals, to those lacking team synergy, and to those lacking alignment with DOE goals. PMs took appropriate actions following external reviews and, when necessary, corrections were made.

1. The ANL Foundational Genomic Science SFA had a PI change in 2015 and had an external review in 2015 and again in 2016. The reviews appeared to have been thoughtfully carried out with multiple opportunities for the SFA to meet the standards for continuation.
2. The Foundational Genomic Science SFAs at LBNL, Los Alamos National Laboratory (LANL), and ORNL had Triennial Reviews in 2014, 2015 and 2015, respectively, which were expeditiously performed, and continuations were recommended with the ranking of "Accept."
3. The Foundational Genomic Science SFA of the Pacific Northwest National Laboratory (PNNL) did not fare well during its 2015 Triennial Review. Two changes in leadership and external reviews were carried out. Clearly, the PMs are providing adequate chances for the SFAs to meet the criteria for continued funding.

Biofuels. In 2014, additional funds were made available from the ending of the Biofuels SFA at PNNL. (The termination decision for the PNNL Biofuels SFA predated the current COV review period.) Nine National Labs were invited to submit Program Plans and the PMs selected five for full proposals, resulting in LLNL securing the funding. The additional funding provided to the LLNL Biofuels program was apparently the stimulus to refocus this SFA effort. It was not clear to the COV whether the dramatic change in focus was discussed by the PMs and the SFA management. The COV realized that this decision was the result of a merit review, and after the outcome there was considerable the PM-management discussion

The Biofuels SFA of the National Renewable Energy Laboratory (NREL) also had a Triennial Review in 2015, followed by an internal DOE annual review in 2016 that had a positive outcome. This small SFA looked much more like a single-PI project, for which other funding mechanisms might be more appropriate.

Low Dose Radiation. The Low Dose Radiation program (with two SFAs) was terminated in FY 2016; the Radiochemistry program (with four SFAs) is currently in ramp-down phase. The COV was not asked to provide input on these decisions.

Bioimaging. In 2014, funds for imaging research ($7.9 million) were directed by Congress toward technology that could be commercialized in the realm of linking metabolism and phenotypes. Budgets of over $9 million were provided in the subsequent years, 2015–2017. The research was expected to result in outsourcing of capacity rather than additions to DOE user facilities. Owing to the short time between funds becoming available and the expenditure deadline in the first year, a broad-call FOA was not practical. Therefore, pilot projects were started in the first year in four DOE labs. One of the National Lab projects did not pass peer review and was terminated after the pilot year.

Whereas the initial funding of Bioimaging SFAs was treated as non-competitive, funds have arisen unexpectedly at year-end to support an SFA that has been subjected to a competitive process. This was the case for the Mesoscale to Molecules (M2M) pilot program for imaging and measurement technology development in 2014. Requests were sent to the National Laboratories for conceptual M2M Bioimaging pilot project proposals, and eight SC Laboratories responded. With limited time for decision-making, the proposals were subjected to an internal review and the programs selected were then externally reviewed the next year. Concerns were evident in the process. The numerical scores from the internal reviews showed that some statistical treatment would have increased confidence in the decisions. The scores could easily have been "truncated" or winsorized (by applying a transformation of statistics to limit extreme values) to obtain a mean for comparison such that a single outlier would not skew the decision. Decisions made during the white-paper evaluations have long-term effects on who is invited to participate in the next year's competition and who gains a competitive advantage by having access to pilot funding. This is a factor that PMs need to be especially mindful of in the SFA review process. Suggestions to allow external reviews prior to decisions given short turnarounds are provided in greater detail below.

Breadth and Depth of Portfolio and Standing

The SFA portion of the BSSD portfolio covers a broad range of topics in fundamental genomic sciences, including topics relevant to biofuel production. For the most part, the projects are large interdisciplinary collaborative efforts that are at the forefront of science in their respective areas of research. The SFA programs are built around the concept that interdisciplinary teams with a longer time frame of support can undertake complex, multifactorial scientific questions or "Grand Challenges" that could not be productively handled by a smaller group with more focused research directions and a shorter time frame. These programs represent an important mechanism by the DOE for enabling scientific research, and the portfolio of SFA projects generally meets this goal. The SFA projects are grouped into three different categories: foundational genomics, biofuels, and bioimaging.

Foundational Genomics. Five SFA projects are included in this topic area, including projects led by scientists at ANL, LBNL, LANL, ORNL, and PNNL. Most of the projects deal with genomics of microbial systems, covering a range of topics from microbial communities to molecular complexes. Most of the projects have been conducted at a high level and are being recognized both for their contributions to fundamental knowledge and for the new technologies being developed.

Biofuels. Three SFA projects, led by scientists at LLNL, NREL, and ORNL, are currently active. The projects cover a diverse array of topics from neutron scattering imaging of lignocellulose during degradation to molecular studies of the ferredoxin interactome in green algae. The projects are making good progress through application of state-of-the-art methods.

Bioimaging. This is a new SFA program that was established in FY 2014. This program complements and expands the SFA research portfolio. Seven projects in this program were financially supported during the time frame covered by this report. These activities were distributed among Ames Laboratory, ANL, BNL, ORNL, PNNL, and SLAC National Accelerator Laboratory. The scientific quality and breadth of the supported programs is notable. These projects focus on a wide range of imaging modalities, are collaborative and interdisciplinary in nature, and make use of and develop modern techniques and approaches.

General Comments

1. The panels for evaluation of SFA programs have been composed of external reviewers with appropriate expertise and numbers for the programs being evaluated.
2. The SFAs in the portfolio are led by outstanding PIs with strong teams of scientists that are experts in the areas needed for conducting the research.
3. The COV recognizes and appreciates that BSSD PMs have been willing to make hard decisions about the quality and efficacy of the SFAs and have ended several programs that were not meeting expected merit standards or maintaining relevance to the BER objectives. These actions have been necessary for maintaining the excellent scientific scope and standards of the overall BER portfolio.
4. There are examples of SFAs that received rather strong criticisms in reviews but that were ultimately funded after discussion by the PMs. This has generally been a successful tactic, with redirection and quality team building leading to a strong SFA in later reviews. Again, the COV appreciates the effort that has been expended in this area and its importance to the overall success of the BER program.

Recommendations

1. The COV strongly valued the summaries provided with respect to the timelines of the SFAs and the decision processes on the cases that did not follow the established

trajectory. The COV recommends that these summaries be made available, where possible, in future COV reviews.

2. In a number of the SFA proposals, the long-term goal or the Grand Challenge addressed was not always evident. Since the National Laboratory interdisciplinary teams were established to address more difficult research projects that could not likely be successfully completed in a single-laboratory setting, the "Grand Challenge" should be evident in each plan.
3. Numerical scores for proposal evaluations should be subjected to an appropriate statistical treatment before ranking, and panels should be provided time for discussion of proposal scoring to adjudicate the decisions. To avoid the necessity of having an internal review on short notice, the COV suggests that BSSD develop a plan to perform an accelerated and consistent adjudication of proposals, preferably including external evaluation of proposals. One of the suggestions to accomplish that goal is to maintain a standing pool of external reviewers willing to do reviews on short notice.
4. Since the M2M imaging program is primarily focused on technology development, that aspect should be better addressed in the proposals. For proposals where a technology is expected to be the objective of the research, the COV recommends that the initial request for white papers or pre-proposals address plans for dissemination and licensing of the resulting technology, if appropriate. Further, developing additional expertise in, and links to, the commercialization process may be useful in aiding potential translational or commercialization opportunities.
5. The COV recommends careful consideration of SFA leadership to ensure that all the SFAs have suitable and inspired directors with sufficient time to devote to project management. The COV also notes that distribution of the leadership roles may generate potential opportunities for other team members—including junior scientists—to assume leadership responsibilities.

D. Funding Opportunity Announcements to the University Community

Overview, Findings and Comments

The work of the COV to evaluate the processes associated with grant solicitation, review, and funding was facilitated by summary sheets prepared by the PMs. The COV also interviewed relevant staff as necessary, analyzed FOAs, and surveyed selected submitted and funded proposals and the related documentation. The BSSD staff and PMs were very helpful and provided substantive additional information during the review process. The COV sensed enthusiasm for and commitment to the mission. The review of materials was greatly facilitated by the PAMS system. Most of the proposals had appropriate documentation in the database, but one was found to lack documentation, possibly owing to a technical error. In addition, helpful summaries of details of each FOA and the review and decision processes were provided in hard copy. Given the 477 project proposals submitted in response to FOAs, the COV could only look at a representative sample and evaluate information for key points under consideration. Proposals

for detailed analysis were chosen either randomly or by some objective criterion (such as place in the scoring range), to avoid any bias. The calls for proposals fell into three categories:

Standard Proposals (initiated by Genomic Science Program Managers):

- *DE-FOA-0001060 (12/20/13), Systems biology of bioenergy-relevant microbes to enable production of next-generation biofuels.*
- *DE-FOA-0001034 (11/19/13), 2014 Plant feedstock genomics for bioenergy: A joint research funding opportunity announcement USDA, DOE (year 1).*
- *DE-FOA-0001207 (10/1/14), Systems biology research to advance sustainable bioenergy crop development.*
- *DE-FOA-0001249 (11/24/14), 2015 Plant feedstock genomics for bioenergy: A joint research funding opportunity announcement USDA, DOE (year 2).*
- *DE-FOA-0001444 (11/4/15), 2016 Plant feedstock genomics for bioenergy: A joint research funding opportunity announcement USDA, DOE (year 3).*
- *DE-FOA-0001458 (11/23/15), Systems biology enabled research on the roles of microbial communities in carbon cycle processes.*

Mesoscale to Molecules (M2M) Bioimaging Technology (Congressionally mandated program)

Initial information about this program and the initiation of pilot projects within the DOE labs was provided above. Subsequently, *DE-FOA-0001192 (9/10/2014), Novel in situ imaging and measurement technologies for biological systems science*, was published. After peer review of submitted proposals and all ongoing pilot projects, seven university-based projects were launched in the second year. Two of these were collaborative with DOE National Laboratories. The COV felt that this process was acceptable under prevailing time constraints, although sufficient time to allow peer review of all proposals submitted after a FOA is publicized is preferred in the future.

Radiochemistry, Imaging Instrumentation, and Nuclear Medicine (Congressionally mandated program)

This program was phased out in an orderly manner in DOE National Laboratories and universities between 2014 and 2016, with gradual reduction of budgets before elimination, which COV commended as allowing easier transitions for grant personnel.

Timing, generation of content, and clarity of the funding opportunity announcements. The mission of BER is defined by Congress, and the COV concluded that the FOAs written in the BSSD program are consistent with the broad mission. The PMs are responsible for formulating FOAs with input from the scientific community and other governmental research offices. Specifically, periodic workshops are held to generate publicly available information highlighting emerging research challenges. Workshops held in this reporting period focused on sustainability (2013), lignocellulose (2014), and molecular sciences challenges linked to geochemistry (2015).

In addition, a multidisciplinary genomic sciences meeting is held annually. Further input is gathered informally at scientific meetings attended by the PMs. BERAC also makes suggestions regarding FOAs that may be implemented, such as, for example, the sustainability initiative. FOAs are also informed by interactions with other Federal funding agencies, both as formal collaborations (e.g., the joint USDA-DOE initiative in feedstock genomics) and informally through interagency meetings.

In response to the recommendation of the 2014 COV, the BSSD made a strong and generally successful effort to develop more focused FOAs. Only one FOA was viewed as overly broad with respect to biological systems and technologies of interest. More focused FOAs were thought to be helpful to those submitting proposals as well as to the reviewers. More focused FOAs also provide a tool for PMs to diversify the BSSD research portfolio by targeting areas not well-represented among funded projects. The COV supported the inclusion of statements about the types of research that were not appropriate for the FOA because these statements added additional clarity. On the other hand, overly focused FOAs may risk excluding research that is potentially important and relevant to the BER mission. The COV noted that duration of prospective awards described in the FOAs was well matched to the nature of the research. This illustrates that the PMs are sensitive to the needs of various types of research programs.

Use of pre-proposals. The COV supports the current practice of using pre-proposals to reduce the overall workload on proposers and reviewers. Currently, pre-proposals are screened solely by the PM using the single criterion of whether the goals of the pre-proposal are consistent with the FOA. There is no peer review for technical merit at this stage, and the COV suggests that the currently used feedback language be changed to make this clear. The pre-proposal process seemed to be effective in eliminating a significant number (e.g., 46% in one case) of proposals from full review. Even so, some FOAs attracted a large number of pre-proposals that matched the strategic goals, resulting in a large number of submitted full proposals that were out of proportion to the dollars available. Such a scenario sets up an unusually low success rate, with significant effort by all parties invested in writing and review of non-funded proposals. PMs reported that currently about 7% to 20% of full proposals submitted are funded. FOAs with the lowest funding rates may discourage PIs from submitting in response to future BER calls for proposals, representing a long-term disadvantage to the mission. The COV recognizes that this concern is not limited to this program, instead reflecting current trends in research funding across multiple agencies. However, if resources and time allow, the PMs could consider panel reviews of pre-proposals for technical merit, with only highly meritorious ones being invited for full proposals. This practice would further reduce the proposal-writing burden on the scientific community by ensuring that a reasonable percentage (e.g., at least 20%) of full submissions are funded.

The COV noted that the time between release of FOAs and due date of the pre-proposals ranged from four to seven weeks. In three of six cases, this time was inclusive of the major holiday period in December/January. The time available after “encourage/discourage” to write and submit a full proposal was three to eight (typically six) weeks, and in one case this time period

also included the major holiday period in December/January. These relatively short turnaround periods, especially those including holiday periods when universities are on break, may work against a broad base of applications. It can be noted that the condensed scheduling for some FOAs was caused by late Congressional action on the budget and was beyond the control of the PMs.

Selection of reviewers. The type of expertise reviewers brought to the panel was documented in DOE-BSSD records provided for COV evaluation. The COV judged that the panels were composed of recognized and respected experts in their fields. Reviewers had diverse and multidisciplinary expertise appropriate for the scope of the FOA and the nature of the anticipated full proposals in the pool. The COV noted appropriate diversity in terms of factors such as stage of career, work sector, and geographic location of the reviewers. In only one case, the reviewer's expertise may not have been entirely consistent with the type of research requested in the FOA, which in turn may have impacted the type of proposals receiving the highest scores. The COV suggests that PMs always strive for a majority of panelists whose research matches the intent of the FOA, in order to achieve the best possible match between the FOA and proposals finally funded. In general, the COV judged that the PMs are doing a good job of soliciting and recruiting qualified reviewers, as well as documenting reasons why some contacted potential panelists declined the invitation. The acceptance of invitations by most people without scheduling conflicts is an indicator of broad-based respect for the grant programs and the role that they play in the advancement of national bioenergy-related research. Review panel sizes are adjusted on the basis of the length and expected number of submissions in response to an FOA. The PMs are commended for being sensitive to reviewer workload, and higher-quality reviews result when reviewers are not overloaded. In addition to the on-site review panel, some proposals with unique research approaches are reviewed by remote panelists who either send in written reviews or engage in a teleconference with the on-site panelists. The COV believes that this is a good approach in concept, making travel unnecessary for someone with special expertise relevant to only a few proposals. Further comments about how this impacts the scoring system appear below.

Review process, decision on awards, and communicating decisions to PIs. Reviewers complete the scoring of proposals assigned to them before meeting for the on-site panel. The composite scores for proposals in any one FOA were widely distributed within a 10-point range, which indicates that reviewers typically exhibited discernment about the quality of the proposals. The spread of each reviewer's scores is available to the PMs as an aid to making final funding decisions. There is substantial discussion of proposals in the face-to-face meeting of the panel. Reviewers may, at their own discretion, change their initial scores as a result of discussion, and any panelist may write a review of a proposal not initially assigned to him or her. Reviewers may comment on any proposal, regardless of initial score. A consensus is not sought from the panel, which is only advisory to the PM, following rules that govern this program.

The COV noted that some proposals with lower scores were described by reviewers as containing high-quality science from well-qualified teams, but having some weaker factors such

as preliminary data or integration within the team. This observation illustrates the competitive nature of this program, with many more scientifically meritorious proposals being received than can be funded. Analysis of the review comments on selected proposals showed that comments were typically consistent with numerical scores, However, in one FOA, there were cases where scores and comments on funded and non-funded mid-ranked proposals did not seem completely consistent.

The COV felt that the Review Panel Managers were generally doing a good job of balancing scores, discussion, written comments, and portfolio balance in making final award decisions. In most cases, the need to balance multiple parameters was evident because the awards did not strictly follow the order of numerical ranking. In cases of funding vs. not funding of proposals with the same numerical score, COV members felt that the factors recorded in the comments, such as enthusiasm and consensus of reviewers, typically supported the decision. For one FOA, the awards were made by strict order of the ranking, but the COV does not have information about the basis for this atypical case. The COV discussed the impact of mean scores derived from typically three, but variable, individual reviewer scores and makes recommendations below for improvement of the process.

The PM makes the final decision on awards and is not bound by the numerical ranking. Factors that sometimes resulted in funding of a lower-ranked proposal while a higher ranked one was not funded included the following: (a) perception of strong disagreement between reviewers that led to a lower numerical ranking than the majority opinion; (b) a reviewer who did not use a broad scale across multiple reviews assigned to him or her; or (c) the need to balance the overall research portfolio. For selected proposals analyzed in detail, the committee felt that the overall comments on funded awards were consistent with the final decision made by the PM.

The reviewers' comments are returned to the PIs, after any essential redaction of non-transmittable comments or identifying information by the PM. The COV believes that this practice is appropriate, providing as much detailed feedback as possible. Scores are not returned to the PIs; the COV finds this appropriate, given that as few as three individual scores are often averaged and the scores are only advisory to the PM. The PM also writes a summary of the discussion after the review process is completed, and it is helpful that this is also returned to the proposer. The COV learned that laws governing BSSD operations (the Federal Advisory Committee Act) prevent a summary provided by the review panel from being generated and provided to the proposer.

Monitoring and disseminating results of funded projects. The annual reporting system in PAMS was identified by the committee as one of the major successes in process optimization during this reporting period. The annual reports now have a uniform format, with tangible and useful information on progress toward meeting the objectives, products of research, and future directions. The reports are linked to the project on-line. The system also allows for the PI to submit more detailed supplemental reports that are not limited in format, and which add to the depth of information.

The OSTI database provides an on-line source of publications from the funded projects, particularly those of National Laboratories, which are required to use the system. These are the last author's version, and they may not reflect corrections made during the final publication process, which are necessitated by policies at some journals. The publications are required to be deposited at three-year intervals.

Genomic Sciences: Systems Biology

Breadth and depth of portfolio and standing. The COV viewed the research funded through FOAs as having an essential leadership position in stimulating public-sector bioenergy research in the United States, as well as being on the forefront of worldwide science in this area. These programs are generating the fundamental and applied knowledge that will allow renewable resources to play an ever-increasing role in our national energy landscape. Worldwide impacts are also anticipated because U.S. bioenergy plant species and production processes can be used elsewhere. The funded proposals were led by well-regarded experts, and publications are appropriate for the discipline. Where high-risk/high-reward research was called for in the FOA, the COV saw evidence that such projects were funded. In summary, the COV felt that the funded proposals were of high quality and appropriate for the program. The scope of the funded research projects is available at http://genomicscience.energy.gov/research/index.shtml and is briefly summarized below.

DE-FOA-0001060 (12/20/13), Systems biology of bioenergy-relevant microbes to enable production of next-generation biofuels. This program captures advances in industrial microbial technologies to provide biocatalysts for transformation of lignocellulosic hydrolysates into specialty biofuels and co-products. The fourteen funded projects included genomics, modeling, rapid automated screening, and advanced genetic engineering, as applied to cyanobacteria, bacteria, fungi, and consortia of organisms. Typically, the projects included a fundamental research question, which was predicted to expand the boundaries of metabolic and synthetic biotechnologies.

DE-FOA-0001207 (10/1/14), Systems biology research to advance sustainable bioenergy crop development. Research was targeted toward addressing the complex relationships between bioenergy crop plants, the soil, and associated microbes in variable environments. This necessitates "systems," or multi-faceted, research. Six team projects including numerous investigators and institutions were funded. Research on major bioenergy crops (switchgrass and sorghum) aimed to optimize bioenergy plant growth on marginal land with water and nutrient limitations as well as biotic challenges. Development of multi-scale models, an essential element of integrating complex data, was funded.

DE-FOA-0001458 (11/23/15), Systems biology enabled research on the roles of microbial communities in carbon cycle processes. This program aims to advance the understanding of global biogeochemical cycling, particularly carbon, and its dependence on microbial

communities. To uncover the nature and magnitude of these microbial processes, diverse technical approaches were funded, including linking ecosystem-scale biogeochemical process with functional activities of microbial and plant communities; extending systems biology approaches to more complex microbial communities; and applying and developing comprehensive and multi-scale techniques for quantitative imaging and analysis of microbial community function.

The Plant Feedstock Genomics for Bioenergy Program

This joint effort of USDA and DOE was defined by three annual FOAs in this review cycle. (Year 1) *DE-FOA-0001034 (11/19/13)* requested "genomics based research that will lead to the improved use of biomass and plant feedstocks for the production of fuels such as ethanol or renewable chemical feedstocks," with special interest in improvement of crop outputs and sustainability; (year 2) *DE-FOA-0001249 (11/24/14)* emphasized "improved resistance/tolerance to disease"; and (year 3) *DE-FOA-0001444 (11/4/15)* extended the call to stress resistance in the field. Twenty-two proposals were funded over three years, and these were focused on improving diverse bioenergy crop plants and developing robust production systems. This program played a unique and critical role in enabling high-quality bioenergy research by smaller research teams, as contrasted with the large-scale BRCs.

DE-FOA-0001192 (9/10/2014) Novel in situ imaging and measurement technologies for biological systems science. The funded projects in this program were diverse, including research in a variety of different systems from soil to pure cultures. Some fairly high-risk research was funded in an effort to push the boundaries of imaging technology in natural systems.

Recommendations for FOAs in General

1. The PMs should use all possible strategies to gather wide input into the content of FOAs during their development stage. Useful tools may include the following:
    - Gathering input at the annual DOE contractors meeting on any changes in the research landscape.
    - Hosting triennial workshops on schedule, including good representation of early-career investigators.
    - Implementing a public comment period on the FOA language before it is finalized.
    - Traveling to scientific meetings. The COV felt that funds for PM travel to scientific meetings in order to stay current on relevant national and international science was inadequate, and additional travel support is recommended. PMs concurred that being able to attend additional meetings would benefit the program.

2. The COV recommends dual attention to promoting research continuity of effective research groups and to stimulating entry of new researchers into the funding programs.

Recognizing that funding and/or external factors may constrain both goals, the following suggestions were made for further consideration:

- Implement an annual Open Call for pre-proposals in core research areas, following the model of Feedstock Genomics. This practice should increase the level of funded innovative and early-career research as well as increase opportunity for all PIs, including the potential to benefit from feedback before resubmission. A teleconference panel to review Open Call pre-proposals for technical merit is recommended in order to keep funding of full proposals at a reasonable percentage.
- Allow up to two additional pages in all full proposals, one to describe the recent BER-funded research and outcomes of the team (if relevant) and a second to describe the qualifications and integration of the research team.
- Whenever possible, pre-proposals should be due eight weeks after the FOA is released, and full proposals should be due at least ten weeks after the "encourage/discourage" notification, with all time intervals excluding ten days in December/January when universities are often closed. This change is predicted to encourage a broader base of applicants, including new investigators.

3. The COV recommends modifications of the scoring system to promote objectivity, fairness, and transparency. In general, we felt that the current process has mainly led to appropriate decisions, but that improvements could be made. Several ideas were discussed for further consideration by the PMs:
    - Provide additional information to reviewers about the appropriate framework for assessment of proposals, including the meaning of the numerical range and the value of scoring across a broad numerical range. Create an automated system to inform the reviewer of the distribution of their scores before their first-phase reviews are finalized in the PAMS system.
    - Generate a rubric of several key factors that reviewers must score individually as a required part of generating the composite score. For example, scientific and technical merit, appropriateness of approach, and team qualifications are core factors. Societal, environmental, and/or educational factors could be added as appropriate for a particular FOA. This system would better inform PMs about specific strengths and weaknesses of each proposal.
    - Ensure that evaluation of consistency with the FOA or assessment of the budget is provided separately for the information of the PM, but does not numerically contribute to the score.
    - Equalize the number of reviewer scores leading to the averaged ranked score, e.g., at three. Any additional perspectives from external reviews or other panelists should be entered in words to aid PMs in making final decisions.
    - Consider normalization of the composite scores for the proposal to the scoring range of each reviewer (e.g. Z-scores). This process would increase the fairness of evaluating ranks of scores with only three inputs and make the current subjective judgment of the PMs on the overall reviewer scoring range more objective. In the

COV's view, such a change is important because it is almost unavoidably more difficult for an initially lower-ranked proposal to be chosen for funding.
    - Provide an explanation (written by the PM) in the Internal Comments section of PAMS when higher-scoring proposals are skipped or choices are made between multiple proposals with the same score. This practice will create more transparency and a permanent record.

4. The COV recommends further attention to dissemination and assessment of publications and other outputs arising from the funded research, as follows:
    - The requirement that all BER-funded publications acknowledge the grant number should be solidified and monitored. This practice will facilitate text searches in standard on-line scholarly databases where final versions of manuscripts are linked.
    - All BER-funded publications should be deposited in OSTI no later than six months after their acceptance for publication. Similarly, links to published patents should be provided there.
    - The Internal Comments section of PAMS should contain a notation on awarded proposals that the PM views as high-risk/high-reward. Over time, meta-data can be generated indicating whether or not this initial prediction results in special project outcomes, e.g., high-profile publications and patents.

Systems Biology Knowledgebase

Overview, Findings and Comments. The ultimate goal of DOE's KBase is to provide the computational environment needed to address the grand challenges of systems biology: predicting and ultimately regulating and even designing biological function. In order to achieve this excellent and ambitious goal, KBase has to integrate and/or develop software tools necessary for interdisciplinary genomic science, including molecular biology, systems biology, and genomics. Detractors may suggest that this project is not scientifically exciting or cutting-edge, but such a large, potentially high-impact project should have a significant service/outreach component to ensure that the system is working well and used by the scientific community. This significant outreach and widespread use can be achieved by implementing a "one-stop" computational resource that is well integrated with other DOE user facilities, like the JGI.

KBase was created as a consortium between four DOE entities: LBNL, ANL, BNL, and ORNL. Initially, KBase was funded through the SFA mechanism, which provides the oversight necessary for tight collaboration and eliminates redundancy between four geographically dispersed programs. However, KBase, the single SFA on this topic, did not fit well into the Computational Biology portfolio because of the different challenges posed by these activities. During the period covered by the COV, the SFA was converted to a project with the hope that this administrative change would provide the flexibility needed for the scientists to respond to user concerns and meet the needs of the research community.

The first Triennial Review was held in 2014, and raised a number of concerns. A management plan was put in place that specified revised goals and approaches, with reevaluation in 2015. The 2015 review resulted in harsh criticism by the external reviewers, a recommendation for broad organizational and operational changes, and acceleration of JGI-KBase integration. With a recommendation of "Partially Accept", the budget remained the same, with added requirements of quarterly reviews to track deliverables. It is thus apparent that very significant involvement by PMs (and reviewers) has been needed to ensure that KBase can make a substantial impact on computational biology problems. In addition, other FOA-funded projects obtained funding with the expectation that KBase would provide useful software within the time frame of these grants.

KBase is an excellent program in principle, supporting the BER research programs and providing tools that could facilitate reproducibility of results. Managing such an intense effort at four institutions across the country is difficult with respect to both crafting the technical details and identifying the correct person for each task.

Breadth and Depth of Portfolio and Standing. The KBase investment is large: 48 FTEs are supported by an annual budget of ~$12M. The outcomes of this project investment have seemingly not been significant or impactful. KBase created a web page with somewhat limited functionality. More importantly, the KBase is not well integrated with other resources, not even with the JGI's databases.

The lack of integration shows that sharing of data, tools, and conclusions in a unified, extensible system is at best a few years away. Currently, KBase users can perform large-scale analyses on scalable computing infrastructure. The scientists can use various programs, but it seems that they are not getting adequate guidance as to what programs are best for particular tasks. KBase has around 2000 users, and about 1000 of these were repetitive users, i.e., used KBase for more than one project. This relatively large community of users has produced only 28 scientific publications that cite KBase, and some of these were published as short communications in Genome Announcements. Moreover, the KBase staff has not published a major paper about KBase capabilities or results.

KBase's main goal (i.e., collaborative creation, sharing, and testing of hypotheses about molecular and cellular functions) still seems to be a future vision rather than a near-term objective. During the last few years, it became apparent that progress has been slower than anticipated, i.e., KBase is slow in translating its many good ideas into working software. Many of the KBase milestones have not been achieved, and the reports are vague. The project is crippled by constantly changing priorities, and this is the major reason why some important milestones are have been pushed further out in time.

The BER-BSSD management has taken multiple steps to improve the KBase outcome and has spent extensive amounts of time and funds on the project. Interactions with the PM seem to be well established and frequent, even though the PM is located in Germantown and KBase is in four different locations. In order to provide necessary guidance, BSSD staff has established bi-

weekly conference calls and quarterly reports. A continuing problem for the PM that was already mentioned in the COV report in 2014 is the limitation of one trip per year for the PM site visits. It seems that management of such a large and geographically disperse program requires more frequent visits. The bi-weekly conference calls are an important management tool, but clearly not a substitute for physical visits and conversations that include not only the leadership of every site but also scientists developing specific tasks. Despite the concerted efforts of the PM and other DOE-BER staff, it seems that the leadership of the project does not provide adequate explanation of the project delays, and the necessity for collaborative efforts is addressed very vaguely.

It is clear to the COV that there has been a very significant and challenging need for continued direction by program staff to ensure that KBase remains a mission-oriented project. The BER-BSSD staff input was also essential to the COV's understanding of the extensive management and direction during the evolution of this program.

Recommendations for the Systems Biology Knowledgebase FOA

1. The COV recommends a serious modification of the KBase effort. One approach to consider is a reduction of the scope of work with more emphasis on developing a subset of the analytical components where KBase can be the leader. For example, KBase has made inroads in metabolic modeling and has expertise that could be further strengthened to obtain national and international recognition. Further, many of the SFAs are generating data that could be used to refine metabolic models, with the models used to generate additional hypotheses testable by the SFAs in an iterative process. Perhaps the fact that KBase was reclassified from an SFA to a Project will allow the modifications to be more easily implemented or provide a mechanism for an amicable dissolution of the team.
2. KBase did not function well when first released. Reversing that reputation is extremely difficult. To build credibility, the COV recommends that KBase be encouraged to publish its plans, results and software. Participation in international competitions for software performance might also strengthen the brand name and should be pursued. The on-line links to the KBase site from the National Laboratories' web pages should be fixed and properly maintained. The user base should be expanded beyond the BSSD and the current user base.
3. Another major concern is the geographical dispersion of the KBase project. DOE staff should consider the possibility of limiting the number of locations, or at a minimum rigorously review the relationships among the consortium's institutions to ensure the level of collaboration and cooperation that is expected from this type of project.
4. The COV is concerned with the information that researchers who are DOE Laboratory employees are strongly encouraged to use KBase, and opines that the use should be motivated by the choice of the best resource, not from the DOE's encouragement to use a particular resource. The COV recommends that BSSD, not KBase, conduct a survey of users to independently assess the methodology and performance of pipelines. KBase should also consider partnerships with researchers outside the DOE system.

5. Overall, BSSD management should consider refocusing the efforts, or reducing the funding level to scale back the project, and should put into place key milestones for making a decision on whether to continue funding or not, or to recompete the program. Where does KBase stand in the greater landscape of bioinformatics platforms? Are the organization, vision and personnel of KBase still appropriate to support this program?

V. BIOENERGY RESEARCH CENTERS

An FOA was published on 4/1/16, which resulted in the recompetition of the BRCs and the establishment of one additional Center in 2017.

Overview, Findings and Comments

Three BRCs were funded during the period of this review, for a total of $25 million annually over the last ten years (two cycles, with $250 million total funding). The productivity of the Centers was substantial, including 89 patents, 175 licenses/options, 365 patent applications, 596 invention disclosures, and 2550 publications. This equates to about $98,000 per publication, similar to Research Project Grants (R01) funded by the NIH, with substantial additional productivity reflected in activities related to technology transfer. Some examples of important technological advances include generation of strains of yeast with improved fermentation capacity, crop plants with improved saccharification potential, and the useful redirection of plant polysaccharide synthesis to foster the biofuels industry.

After the on-site COV meeting ended, the Centers were recompeted (sometimes with modifications of focus) and one additional Center was added to the group. Our review focuses on monitoring the progress of the previously funded BRCs. The annual reports of the BRCs were thorough. On-site reviewers were well-qualified scientists with relevant expertise. Their written reviews discussed objective productivity and impact criteria, as well as team interactions and internal data repositories and analytical platforms that are critical for long-term success of large-scale efforts. Consideration was given in Center reports and by reviewers to technoeconomic, life cycle, and/or ecosystems analysis of developing technologies. Reviews were balanced, with both laudatory comments and suggestions for improvement. The overall coherency and goal-directed nature of these large-scale efforts were adequately addressed. Individualized reviews from the panel members, without personal identification, were provided as feedback to Center management.

After review comments were provided to Center management, follow up communications with the PM demonstrated a focus on technological advances, as appropriate for the objectives of these centers. Since annual renewal is not required, the site visits are advisory to the Center and the PM. The PM mentioned expectations of collaboration within and between the Centers, which the COV felt was appropriate. The number of collaborative publications has been increasing as the Centers have matured.

Given the large amount of public funds invested, all BRCs should be monitored and encouraged to collaborate through monthly teleconferences with the PM, and should produce a detailed written annual report; both of these things are currently done. The COV had a specific recommendation about the frequency of site visits. The COV noted the need to make sure that the detailed and frequent review of pre-set milestones does not suppress high-risk science that may especially benefit from transdisciplinary expertise in these large teams.

Breadth and Depth of Portfolio and Standing

The large-scale, transdisciplinary, and multi-institutional BRCs are accomplishing the dual goal of generating knowledge and translating it to useful advances in the private sector. Appropriate breadth and depth is evident in these large programs, bridging from labs to production plants to field experiments, including assessments of environmental, sociological, and economic impacts of new technologies. A diverse array of organisms and approaches are included within the three Centers that were operational during this review period, which greatly enhances the probability of meaningful practical impacts of the funded research on bioenergy sustainability. Transfer of technology to industry commonly occurs in these Centers, demonstrating the applied value of the research.

Recommendations

1. Site visit reviews of the BRCs should occur in years 2 and 4 for those renewed through peer review after at least one three-year cycle of operations. Any newly established BRC should have an annual site visit for the first five years of its operation. The site visits should continue to include external scientific experts, as is currently done.
2. Given the high capacity to make key advances within the BRCs, the PMs should consider a specific review and reward system for meeting high-risk/high-reward objectives. To foster such work, there should be no penalties when management-approved high-risk efforts do not come to fruition as expected.
3. Encourage BRCs to make available summary statements about major experiments that are not being pursued in a continuing manner, but which may represent valuable knowledge for the broader scientific community. An example would be genes tested that did not result in useful technological advances. Such information, including contact information for further questions, would promote overall efficiency in the broader scientific community by diminishing repetitive work.

VI. WORKSHOPS

BER funds workshops and conferences through its Open Call program in consultation between the requestor and individual PMs. Decisions on funding were made internally on the basis of availability of funds and fit with programmatic goals. A variety of conferences and workshops

were supported with funds ranging from $5K to 40K. Several conferences and workshops were supported in 2014–2015. The COV strongly supports this use of discretionary funds, as it provides forums for discussing science and technologies and planning future SFAs and FOAs relevant to the DOE mission.

APPENDIX A: COV CHARGE LETTER

Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 5, 2016

Dr. Gary Stacey
Endowed Professor of Plant Science
Divisions of Plant Sciences and Biochemistry
271E Christopher S. Bond Life Sciences Center
University of Missouri
Columbia, MO 65211

Dear Dr. Stacey:

By this letter I am charging the Biological and Environmental Research Advisory Committee (BERAC) to assemble a Committee of Visitors (COV) to assess the processes used by the Biological Systems Science Division (BSSD) within the Office of Biological and Environmental Research (BER) to manage BSSD research programs and its user facility, the Joint Genome Institute (JGI).

The COV should assess the operations of the BSSD's programs for fiscal years 2014, 2015, and 2016. This includes funding at national laboratories and universities and other activities handled by the program during this time period. It should also assess the quality of the resulting scientific portfolio, including its breadth and depth and its national and international standing. Additionally, the COV should also assess the division's management and oversight of the JGI user facility for the same time period. Specifically, I would like the panel to consider and provide an evaluation of the following:

1. For both the DOE national laboratory projects and university grants, assess the efficacy and quality of the processes used by BSSD programs during the past three years to:
   a) solicit, review, recommend and document application and proposal actions, and
   b) monitor active awards, projects and programs.

2. Within the boundaries defined by DOE mission and available funding, comment on how the award process has affected:
   a) the breadth and depth of the portfolio elements, and
   b) the national and international standing of the portfolio elements.

COV members will be given access to all program documentation completed during the period under review including applications, proposals, review documents and other requests. COV members may also request, at their discretion, that a representative

sample of the program portfolio be provided. In response, BSSD may suggest a sample of actions, including new, renewal and supplemental applications and proposals, awards, and declinations. In addition, COV members may also choose to review files through a random selection process. The guidance for all COV reviews within the Office of Science can be found at http://science.energy.gov/sc-2/committees-of-visitors/ and attachments therein.

The COV should take place in the third quarter of FY 2017 (Summer 2017) at the BER/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A discussion of the COV report by BERAC should be held no later than the Fall 2017 BERAC meeting. Following acceptance of the full BERAC membership, the COV report with findings and recommendations is to be presented to me, as the Director, Office of Science.

If you have any questions regarding this charge, please contact Todd Anderson, 301-903-3213 or by email Todd.Anderson@science.doe.gov.

Sincerely,

C. A. Murray
Director, Office of Science

cc: Sharlene Weatherwax
Todd Anderson
Tristram West

APPENDIX B: COV MEMBERS LIST

2107 COV Reviewers

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APPENDIX C: COV AGENDA

Department of Energy
Office of Biological and Environmental Research
Biological Systems Science Division
2017 Committee of Visitors' Meeting Agenda
July 10–12

Monday, July 10, at Gaithersburg Hilton Hotel (all BSSD staff welcome to attend):

6:00 pm – 7:00 pm Group Dinner in the Darnestown Room at the Gaithersburg Hilton
7:00 pm – 9:30 pm COV Members and BSSD staff in the Darnestown Room

- COV Discussion/Review of Charge Letter/Breakout Groups/Agenda, A. Joachimiak, COV Chair, (20 minutes)
- COV introductions (15 minutes)
- Welcome and BER overview, S. Weatherwax, BER Director (10 minutes)
- BSSD overview (with key points in response to 2014 COV), T. Anderson, BSSD Division Director (45 minutes)
- COV logistics – M. Rutledge (5 minutes)
- PAMS demo – R. Hirsch (15 minutes)
- Conclusions – A. Joachimiak (10 minutes)

Tuesday, July 11 at DOE

7:00 am – 7:45 am Breakfast on your own at the Hotel
7:45 am – 8:05 am Transit to DOE (Shuttle takes COV Members to GTN for admission by Security)
8:05 am – 8:30 am Badging and Security at DOE Front Desk - Transit to meeting room E-401
8:30 am – 9:00 am Executive Session: COV Members
9:00 am – 9:10 am Overview of BSSD, Todd Anderson, BSSD Division Director
9:10 am – 10:00 am BSSD staff short presentations and Q&A

- Genomic Science Program, C. Ronning
- Bioimaging, P. Srivastava
- KBase, R. Madupu
- DOE JGI, D. Drell
- Structural Biology Infrastructure, A. Swain

10:00 am – 10:15 am Break (E-401)
10:15 am – 10:30 am Breakout groups move to separate review rooms

- Facilities group moves to room J-108
- Lab SFA group moves to G-258
- Non-lab FOA group moves to E-164

10:30 am – 12:30 pm Breakout groups begin review of materials (BSSD staff on stand-by)

12:30 pm – 1:30 pm Working Lunch (E-401)
1:30 pm – 3:30 pm Breakout groups continue review of materials (BSSD staff on stand-by)
3:30 pm – 4:00 pm Break (Refreshments provided in Room E-401)
4:00 pm – 5:30 pm Breakout groups continue review of materials (BSSD staff on stand-by)
5:30 pm – 6:00 pm Breakout groups meet with BSSD Staff in Room E-401 (Outbrief BSSD staff/Questions/Requests for Further Information)
6:00 pm – 6:15 pm BSSD Staff transport Reviewers to the Hotel
7:00 pm – 8:30 pm Dinner on your own

Wednesday, July 12 at DOE

7:00 am – 7:45 am Breakfast on your own
7:45 am - 8:05 am Transit to DOE (Shuttle takes COV members to GTN for admission by Security)
8:05 am - 8:30 am Badging and Security at DOE Front Desk - Transit to meeting room E-401
8:30 am - 8:45 pm COV Executive Session
8:45 am – 9:00 am Breakout groups move to separate review rooms

- Facilities group moves to room J-108
- Lab SFA group moves to G-258
- Non-lab FOA group moves to E-164

9:00 am – 10:45 am Breakout groups continue to review materials (BSSD staff on stand-by)
10:45 am – 11:00 am Break (Refreshments provided in Room E-401)
11:00 am – 12:30 pm Breakout Sessions continue review of materials (BSSD staff on stand-by)
12:30 pm – 1:30 pm Working Lunch/Executive Session (Provided for COV in Room E-401)
1:30 pm – 2:00 pm Meeting with BSSD staff
2:00 pm – 2:15 pm Staff transport Reviewers to the Hotel
2:15 pm – 2:45 pm Executive session: Reviewers at Hotel in the Darnestown Room
2:45 pm Meeting Adjournment

APPENDIX D: COV BSSD STAFF MEMBERS AND RESPONSIBILITIES

Name	BSSD Program	Phone Number
Todd Anderson	BSSD Director Radiobiology Research	301-903-5469
Meredith Rutledge	Scientific Program Specialist	301-903-0088
Dawn Adin	Foundational & Analytical Genomic Science	301-903-0570
Dan Drell	Joint Genome Institute – JGI	301-903-4742
Roland Hirsch	Foundational & Analytical Genomic Science	301-903-9009
Ramana Madupu	Computational Bioscience	301-903-1398
Kent Peters	Bioenergy Research Centers	301-903-5549
Pablo Rabinowicz	Foundational & Analytical Genomic Science	301-903-0379
Cathy Ronning	Foundational & Analytical Genomic Science Metabolic Synthesis and Conversation	301-903-9549
Prem Srivastava	Radiochemistry and Imaging	301-903-4071
Amy Swain	Radiochemistry and Imaging Structural Biology Infrastructure	301-903-1828
Elizabeth White	Foundational & Analytical Genomic Science Human Subjects	301-903-7693

APPENDIX E: COV MEMBER ASSIGNMENTS

Dr. Andrzej Joachimiak (Chair)

Group	Program Areas	Materials	Reviewers	Presenters
1	User Facilities Group (JGI, Structural Biology, KBase)	Annual reports Triennial Reviews Operational issues (ITS, CSP review summaries, SB reviews) DOE guidance	Dr. Britt Hedman, G1 Chair Dr. Wladek Minor Dr. Daniel Schachtman	Dan Drell, Amy Swain, Ramana Madupu
2	National Laboratory SFA Group (GenSci, Bioimaging, Plant/Microbio)	BRC Review materials Science plans Annual reports Triennial Reviews Reviewer recruitment Review process DOE guidance	Dr. Ken Keegstra Dr. Lukasz Kurgan Dr. Barbara Methe Dr. Judy Wall, G2 Chair	Cathy Ronning, Pablo Rabinowicz, Kent Peters, Prem Srivastava, Dawn Adin, Ramana Madupu, Roland Hirsch,
3	FOA Group (GenSci, BRCs, Feedstocks, Plant/Microbio)	Notices Pre-app info Proposal list Reviewer recruitment Instructions to reviewers Selection summaries Award/Declination letters Workshops One-off projects	Dr. Zygmunt Derewenda Dr. Bruce Dien Dr. Adam Godzik Dr. Candace Haigler, G3 Chair Dr. Rhona Stuart	Cathy Ronning, Prem Srivastava, Pablo Rabinowicz, Dawn Adin,