

Project Assessment for Biological and Environmental Research

Report from the BER Advisory Committee

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About BERAC

The Biological and Environmental Research Advisory Committee (BERAC) provides advice on a continuing basis to the U.S. Department of Energy's (DOE) Office of Science Director on the many complex scientific and technical issues that arise in developing and implementing DOE's Biological and Environmental Research program (science.osti.gov/Ber/berac).

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Project Assessment for Biological and Environmental Research

Report from the BER Advisory Committee

May 2024

Charge Letter



Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

December 1, 2023

To: CHAIRS OF THE OFFICE OF SCIENCE FEDERAL ADVISORY COMMITTEES:

Advanced Scientific Computing Advisory Committee
Basic Energy Sciences Advisory Committee
Biological and Environmental Research Advisory Committee
Fusion Energy Sciences Advisory Committee
High Energy Physics Advisory Panel
Nuclear Science Advisory Committee

The Department of Energy's Office of Science (SC) has envisioned, designed, constructed, and operated many of the premiere scientific research facilities in the world. More than 38,000 researchers from universities, other government agencies, and private industry use SC User Facilities each year—and this number continues to grow.

Stewarding these facilities for the benefit of science is at the core of our mission and is part of our unique contribution to our Nation's scientific strength. It is important that we continue to do what we do best: build facilities that create institutional capacity for strengthening multidisciplinary science, provide world class research tools that attract the best minds, create new capabilities for exploring the frontiers of the natural and physical sciences, and stimulate scientific discovery through computer simulation of complex systems.

To this end, I am asking the SC advisory committees to look toward the scientific horizon and identify what new or upgraded facilities will best serve our needs in the next ten years (2024-2034). More specifically, I am charging each advisory committee to establish a subcommittee to:

1. Consider what new or upgraded facilities in your disciplines will be necessary to position the Office of Science at the forefront of scientific discovery. The Office of Science Associate Directors have prepared a list of proposed projects that could contribute to world leading science in their respective programs in the next ten years. The Designated Federal Officer (DFO) will transmit this material to their respective advisory committee chairs. The subcommittee may revise the list in consultation with their DFO and Committee Chair. If you wish to add projects, please consider only those that require a minimum investment of \$100 million. In its deliberations, the subcommittee should reference relevant strategic planning documents and decadal studies.

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2. Deliver a short letter report that discusses each of these facilities in terms of the two criteria below and provide a short justification for the categorization, but do not rank order them:
 - a. **The potential to contribute to world-leading science in the next decade.** For each proposed facility/upgrade consider, for example, the extent to which it would answer the most important scientific questions; whether there are other ways or other facilities that would be able to answer these questions; whether the facility would contribute to many or few areas of research and especially whether the facility will address needs of the broad community of users including those whose research is supported by other Federal agencies; whether construction of the facility will create new synergies within a field or among fields of research; and what level of demand exists within the (sometimes many) scientific communities that use the facility. **Please place each facility or upgrade in one of four categories: (a) absolutely central; (b) important; (c) lower priority; or (d) don't know enough yet.**
 - b. **The readiness for construction.** For proposed facilities and major upgrades, please consider, for example, whether the concept of the facility has been formally studied; the level of confidence that the technical challenges involved in building the facility can be met; the sufficiency of R&D performed to date to assure technical feasibility of the facility; the extent to which the cost to build and operate the facility is understood; and site infrastructure readiness. **Please place each facility in one of three categories: (a) ready to initiate construction; (b) significant scientific/engineering challenges to resolve before initiating construction; or (c) mission and technical requirements not yet fully defined.**

Many additional criteria, such as expected funding levels, are important when considering a possible portfolio of future facilities, however, for this assessment I ask that you focus your report on the two criteria discussed above.

I look forward to hearing your findings and thank you for your help with this important task. I appreciate receiving your final report by May 2024.

Sincerely,



Asmeret Asefaw Berhe
Director, Office of Science

BERAC Subcommittee

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Caroline Ajo-Franklin, Co-chair, *Rice University*

Leo Donner, Co-chair, *National Oceanic and Atmospheric Administration*

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Introduction

The construction, operation, and stewardship of large-scale scientific user facilities and cutting-edge capabilities have been integral to the mission of the U.S. Department of Energy (DOE) Office of Science from its earliest days. To help identify and prioritize new or upgraded facilities critical to scientific innovation over the next 10 years, the Office of Science director issued a charge to the federal advisory committees of six of its program offices in December 2023, including the Biological and Environmental Research (BER) program.

The charge letter (see p. ii) asked the advisory committees to:

1. Consider what new or upgraded facilities will be necessary to position the Office of Science at the forefront of scientific discovery.
2. Deliver a short letter report describing each facility in terms of two criteria: (a) the potential to contribute to world-leading science in the next decade and (b) the readiness for construction.

In response to this charge letter, BER's advisory committee (BERAC) established a subcommittee on Project Assessment. As part of this activity, BER provided a descriptive list of nine projects to the 24 subcommittee members for their evaluation. Of the following nine projects, six represent potential user facilities, and three are for Major Items of Equipment (MIE) that may augment or update existing user facilities:

- Microbial Molecular Phenotyping Capability
- Drizzle, Aerosol, and Cloud Observation Chamber
- BER Data Center
- Plant Transformation Capability
- Bioeconomy Accelerator Facility
- Earth System Modeling and Analysis Center User Facility
- EcoPODs and Smart Soil Systems (MIE)
- Visual Proteomics Capability (MIE)
- Phased Array Radar (MIE)

The subcommittee—chaired by Dr. Himadri Pakrasi and co-chaired by Drs. Leo Donner and Caroline Ajo-Franklin—assigned two subject matter experts to each project to help assess its scientific need and impact. Five meetings were held between January and April 2024. The first meeting introduced charge materials. In the second, third, and fourth meetings, subject matter experts gave presentations and led discussions about each project (three per meeting). The final meeting summarized findings and provided additional time for discussion and clarification. The subcommittee presented its final conclusions on April 12, 2024, at the spring BERAC meeting. This report discusses those conclusions, detailing the subcommittee's evaluation of each project based on the questions posed in the charge letter.

Microbial Molecular Phenotyping Capability

Construction Project • Total Project Cost Range: \$100 million to \$167 million

Project Description

The Microbial Molecular Phenotyping Capability (M2PC) will provide unique automated and high-throughput capabilities within a current BER user facility (Environmental Molecular Sciences Laboratory) to phenotype vast numbers of microbial isolates, providing crucial functional data on microbial communities from a wide variety of environments. This facility upgrade achieved Critical Decision-0 in FY 2021 and Critical Decision-1 (CD-1) in FY 2024.

The M2PC project will design and construct a new capability that will provide a range of wet chemistry and instrumentation spaces conducive for highly autonomous operations, as part of an Office of Science User Facility. The project will include acquisition of analytical instrumentation and microbial culturing and characterization capabilities that will be modular and expandable, self-contained, and operate in an automated pod configuration.

Recent advances in computational analysis combined with automated instrumentation and miniaturization have progressed to the point where broad-scale phenotyping of large numbers of varied microbial isolates is now possible. What has historically been pursued on an individual microorganism basis can now be carried out on thousands of microorganisms at once and to a level of genomic/omic detail not previously possible. The need for this capability was highlighted in the *Grand Challenges for Biological and Environmental Research* report (BERAC 2017).

Potential to Contribute to World-Leading Science in the Next Decade

A *Absolutely central*

B Important

C Lower priority

D Don't know enough yet

Readiness for Construction

A Ready to initiate construction

B *Significant scientific/engineering challenges to resolve before initiating construction*

C Mission and technical requirements not yet fully defined

Overall Assessment

The BERAC subcommittee finds that M2PC is essential. Overall, M2PC has a high potential to contribute to world-leading science in the next decade. It would phenotype vast numbers of microbial isolates, providing crucial functional data on those communities from multiple environments, a goal highlighted in the BERAC Grand Challenges report (BERAC 2017). This makes the scientific importance of M2PC absolutely central. However, significant unanswered questions remain regarding how M2PC will operationally meet its mission of covering diverse consortia and environmental conditions. Significant scientific engineering challenges thus exist with respect to construction readiness.

Scientific Importance

Microorganisms represent the largest amount of biomass on Earth and play vital roles in ecosystem function and biogeochemical cycling. Advances in nucleic acid sequencing have revealed that microbial consortia likely harbor immense but undiscovered biochemical capacities. Efforts to discover this biochemical capacity have consistently lagged behind the scientific community's genetic understanding of microbial communities. This gap is particularly wide for microbes that play a major role in DOE-relevant processes. Addressing this challenge requires filling a major unmet need for high-throughput, systematic approaches that leverage laboratory automation and integration to study genotype-phenotype relationships across microbial consortia and environmental conditions.

No existing facilities address this need at the scale required to make significant progress. Additionally, because of its expertise and leadership in the genomic revolution, DOE is uniquely qualified and positioned to develop such a facility. If M2PC could dramatically improve the understanding of genotype-phenotype relationships across diverse microbes, this new knowledge will have far-reaching implications across water, food, energy, environment, and human health. The ability to generate this knowledge likely will create new synergies, not just in microbial biology but also in research to advance the bioeconomy and biomanufacturing. Thus, M2PC is deemed absolutely central.

Construction Readiness

The need for M2PC has been articulated and assessed. M2PC has been approved at the CD-1 level in FY 2024.¹ Conceptual drawings have been developed; they include space for process development, sample preparation, and a 12,000-square-foot automated laboratory within a larger 24,500-square-foot facility. These are important steps toward construction readiness.

The BERAC subcommittee identified two major scientific engineering challenges related to construction readiness. First, M2PC will need to develop technical solutions and scientific strategies to enable cultivation of consortia across a vast, diverse biological and environmental (conditional) parameter space. Current estimates suggest only 1% of microbes can be cultivated; M2PC aspires to significantly increase this percentage for microorganisms representing all three domains: bacteria, archaea, and eukaryotes. Additionally, the parameter space for cultivation conditions is enormous: oxygen, pH, and temperature combined with different carbon, nitrogen, and phosphorus sources. It is unclear what solutions beyond cultivating consortia will be used to address this vast challenge. Second, M2PC will need to assemble all the equipment infrastructure and state-of-the-art technologies necessary to quickly perform genomic, metatranscriptomic, metaproteomic, metabolomic, and secondary metabolite analyses. How M2PC will overcome both these challenges remains unclear.

Recommendation

As DOE moves forward with M2PC, incorporating the agency's existing investments and relevant expertise will be important in M2PC development. Other groups at DOE national laboratories have invested in capabilities that could move toward the development of a high-throughput characterization capability for genotype-phenotype relationships and microorganisms in different environments.

¹ The Office of Science requires that a series of high level, Critical Decisions (CDs) be made in order for a project to advance: **CD-1: Approve Alternative Selection and Cost Range.** One of the alternatives proposed in the CD-0 is selected, and a credible cost range is established.

Drizzle, Aerosol, and Cloud Observation Chamber

Construction Project • Total Project Cost Range: \$34 million \$47 million

Project Description

The Drizzle, Aerosol, and Cloud Observation (DRACO) Chamber is an experimental facility for controlled testing of cloud and aerosol processes. This facility upgrade achieved Critical Decision-0 (CD-0) in FY 2023 with CD-1 planned for FY 2026. Construction would include either a new building or renovation of an existing building to house the chamber, specialized temperature/pressure/humidity controls, and development of instruments and software to characterize the chamber. The ability to address fundamental questions about aerosol–cloud–precipitation interactions is currently limited by the lack of appropriate laboratory cloud and aerosol research facilities of the scale and type needed. A convection chamber with a vertical extent of at least 10 m that can develop and maintain turbulent flows in a supersaturated environment is required to study the full droplet growth process from activation to vapor condensation to collision-coalescence to drizzle onset; the impact of entrainment mixing on these processes; and the evolution of these processes in steady-state conditions.

The proposed chamber would fill critical gaps in the ability to study processes of entrainment mixing, collision-coalescence, and drizzle initiation that are necessary for fundamental scientific understanding of aerosol–cloud interactions and that cannot be studied in existing cloud chambers. The facility would provide the information needed for development of next-generation, physically based parameterizations for microphysical processes in cloud and climate models, increase process understanding to inform marine cloud brightening studies, and reduce uncertainties in hydrometeor remote sensing in the atmosphere. The research conducted in this facility will greatly enhance BER’s international leadership in aerosol and cloud microphysical processes and aerosol–cloud interactions and international leadership in laboratory chamber facilities as identified in the *U.S. Scientific Leadership Addressing Energy, Ecosystems, Climate, and Sustainable Prosperity* report (BERAC 2022) and the *Scientific User Research Facilities and Biological and Environmental Research* report (BERAC 2018).

Potential to Contribute to World-Leading Science in the Next Decade

- A** Absolutely central
- B** Important
- C** Lower priority
- D** Don’t know enough yet

Readiness for Construction

- A** Ready to initiate construction
- B** Significant scientific/engineering challenges to resolve before initiating construction
- C** Mission and technical requirements not yet fully defined

Overall Assessment

The BERAC subcommittee finds the DRACO Chamber is absolutely central but only if it is part of an Aerosol and Cloud Observation facility (ACO), a more comprehensive facility addressing fundamental questions in cloud microphysics important to understanding clouds in the Earth system. ACO would be a multifaceted facility to address long-standing knowledge gaps over a wide range of cloud-aerosol-precipitation processes that cause leading uncertainties in climate models. The facility would include (1) a combination of laboratory-scale wind tunnels and chambers and a suite of associated bench-top ready instrumentation with broad capabilities to characterize observed conditions, conduct a large array of experiments, and host guest instruments; (2) an instrument development arm to focus on long-standing measurement challenges, better characterize existing instruments, and promote technology transfer to operations; and (3) a facility-based modeling capability, necessary to understand and synthesize facility experiments, promote rapid movement of facility results into models, and promote community engagement in reducing process uncertainty. This facility, with a total cost of about \$100 million to \$120 million for all components, would be nothing short of transformational for laboratory microphysics.

Scientific Importance

The BERAC subcommittee concurs that science questions related to drizzle and aerosol processes, especially if studied in the context of turbulence, are important. While interactions between turbulence and microphysical processes (ranging from activation through collision-coalescence and drizzle initiation) are critical, they are of lower priority in contrast to less-resolved, high-impact questions regarding ice microphysics. Inability of atmospheric models to represent ice processes is one of the most significant contemporary issues impeding climate research and prediction. Cold cloud processes lack convergent understanding across the community, including primary and secondary ice production processes and reproducibility of laboratory studies. A forthcoming 2024 BER Atmospheric Ice

Processes Research report concludes there is a pressing need for a national facility to undertake cloud ice processes and physics research, including mixed-phase. The facility should be centered around chambers and wind tunnels, including bench-scale experimental and instrument development capabilities, and directly integrate modeling work. The BERAC 2022 international benchmarking report called for an aerosol–cloud laboratory facility, though in more general terms (BERAC 2022). The BERAC 2018 user facility report called for development of “new technologies” to address aerosol–cloud needs, specified ice formation as an area in need of “transformational advances in understanding,” and identified the need for laboratory chambers to address cold cloud processes (BERAC 2018).

These reports convey the urgency with which BER has recognized the need to develop an ACO laboratory facility and emphatically emphasize the necessity of constructing a facility that not only enables study of drizzle processes but ice processes as well. Limiting the facility to drizzle and warm processes would fail to realize fully the enormous potential of this facility, the importance of which BERAC identifies as absolutely central. A comprehensive facility including warm and cold cloud processes with turbulence would be unique, providing DOE with next-generation leadership in laboratory studies of clouds. ACO would put DOE at the forefront of scientific discovery at a time of great need in the modeling community. The German user facility at the Karlsruhe Institute of Technology demonstrates the value of synergy in hosting two large chambers, guest instruments and experiments, advanced bench-scale facilities, and instrument development. However, the user facility has no vertical wind tunnels suitable for studying multi-hydrometeor interactions with precipitating ice, has no modeling arm, and stands alone in its class.

Construction Readiness

Significant scientific and engineering challenges remain before initiating construction for the DRACO elements (drizzle and aerosol processes in the presence of turbulence). In particular, designing the DRACO Chamber so the character of the turbulence

it generates faithfully replicates turbulence in cloudy atmospheres will be important. BERAC translates this to a (B) readiness rating for the DRACO component of ACO. The ice, mixed-phase, and precipitating components of ACO require further scoping and design. These components of ACO would expand on previous wind tunnel and chamber designs, along with new, cutting-edge approaches. These ACO components are at a (C) readiness level, not yet fully defined. DRACO achieved CD-0 status in FY 2023.²

² The Office of Science requires that a series of high level, Critical Decisions (CDs) be made in order for a project to advance: **CD-0: Approve Mission Need.** A determination is made that there is a scientific case to pursue the project. Some of the possible alternative means of delivering the science are presented as well as a coarse estimate of the cost.

Recommendation

The recommended ACO components, DRACO among them, are as described above. Design review for DRACO is recommended. While recommendations regarding this facility stand independently of the status of other facilities under consideration in response to this charge, BERAC notes that the proposed phased array radar (see p. 20) would transform opportunities to interpret field observations using an all-phases chamber including turbulence. Bridging laboratory and field observations in this way would provide powerful synergy in understanding clouds.

BER Data Center

Construction Project • Total Project Cost Range: To be determined

Project Description

The BER Data Center is envisioned as a centralized data and mid-range computational infrastructure for tackling the data challenges of BER's biological, Earth, and environmental research programs. The volume and rate of BER-generated data are growing exponentially due to improvements in instrument resolution, advances in laboratory automation, and increased model complexity. BER's focus on systems science leads to the creation of data that span across molecular to global spatial scales; nano-seconds to decadal temporal scales; and experimental, observational, and computational sources. Integration of these heterogeneous data sources is essential to address BER's systems science focus and scientific grand challenges. Thus, there is a need to develop either a centralized data computational infrastructure or interconnected data stores that are integrated with mid-range computing capabilities to support complex workflows for analysis and simulation as well as archiving, managing, and visualizing experimental, observational, and model data along with metadata.

A BER data facility will promote harmonization of data management and analysis services (including the use of artificial intelligence and machine learning approaches) across BER's diverse scientific community, which ranges from molecular biologists to Earth system modelers. The facility will enable BER-supported researchers to easily schedule and use different infrastructure capabilities; support the integration and management of models, experiments, and data across a hierarchy of scales and complexity; and accelerate the pace of scientific discovery and predictive understanding of biological systems and Earth systems. The purpose of this facility is not to replace existing BER data resources but rather to serve as an integrating hub, expediting data sharing across multidisciplinary teams of researchers and enabling development of collaborative workflows. The data center will coordinate data management, mid-range computing resources, and analysis efforts at BER-supported facilities and across large programs, as well as develop new capabilities, to create an integrated data and mid-range computing facility that facilitates the analysis and synthesis of data for complex and multidisciplinary research efforts across BER. The need for this capability was highlighted in the *Scientific User Research Facilities and Biological and Environmental Research* report (BERAC 2018).

Potential to Contribute to World-Leading Science in the Next Decade

- A** Absolutely central
- B** Important
- C** Lower priority
- D** Don't know enough yet

Readiness for Construction

- A** Ready to initiate construction
- B** Significant scientific/engineering challenges to resolve before initiating construction
- C** Mission and technical requirements not yet fully defined

Overall Assessment

The subcommittee recognizes the need for a BER Data Center (BDC) for BER stakeholders whose research activities range in spatial dimensions from atomic to planetary distances and in temporal dimensions between subseconds to millennia. However, the concise proposal above lacks important details necessary to assess the scope and construction readiness. In addition, the DOE Advanced Scientific Computing Research program (ASCR) is planning to develop a large data center to serve the needs of all DOE Office of Science scientists. The BDC should work closely with ASCR to avoid duplication and to take advantage of DOE infrastructure as well as ASCR methodologies. The subcommittee's overall recommendation is to establish a BDC after its overall scope has been defined in detail.

Scientific Importance

The BERAC subcommittee places the BDC in the category of (A) absolutely central. Biological systems and Earth system processes are unavoidably coupled. Biological processes, whether harbored in microbes, plants, or human populations, can significantly affect global elemental cycles and climate dynamics and are, in turn, dramatically affected by environmental changes at multiple scales. Scientists from different disciplines have collected enormous amounts of diverse data that are helpful for understanding these processes.

These data are collected using diverse technologies by scientists trained in very different disciplines and stored in different facilities. Yet, many important and urgent questions related to sustainability and global change cannot be addressed without a long-term, democratized way to concurrently access and process these different types of data. Proper storage, annotation, and distribution of data is a fundamental enabling technology that can support efforts to build quantitative models that in turn can integrate these data and generate predictions of possible scenarios and interventions.

Construction Readiness

The BERAC subcommittee places the BDC in the category of (C) mission and technical requirements not yet fully defined. Details relevant to this proposal have been discussed extensively in the 2024 BERAC report *A Unified Data Infrastructure for Biological and Environmental Research*, especially with respect to assessing existing infrastructures and their accessibility as well as exploring grand challenges that could be pursued by decreasing existing barriers for data access and integration (BERAC 2024). The BERAC subcommittee recommends that the following challenges and concerns be addressed in a more detailed proposal for the BDC: (1) data diversity and challenges of an integrated infrastructure, (2) roles of and impacts on existing resources, (3) expertise and leadership, and (4) possible avenues for technical implementation.

Plant Transformation Capability

Construction Project • Total Project Cost Range: To be determined

Project Description

The Plant Transformation Capability (PTC) is intended to become a new capability to be added to an existing facility (e.g., Joint Genome Institute) to develop robust and cost-effective plant transformation capabilities for bioenergy feedstocks. Using the latest genomic-enabled biotechnology, this capability will provide new ways to work with and design new crops with added beneficial traits for a variety of useful economic purposes. While the science for genome engineering of microbial systems is advancing rapidly, significant bottlenecks exist when it comes to unlocking a similar potential for plants to fully harness the benefits of a burgeoning bioeconomy. Current transformation methods are highly germplasm dependent making them challenging for bioenergy crops, and current processes are very labor-intensive requiring specialized hands-on training and specialized expertise, which is dwindling due to retirements in the field.

This new capability will develop the needed techniques based on new biotechnology tools to accelerate the ability to efficiently design and genomically transform plants for a range of bioeconomic purposes.

Plants are complex organisms with complex traits associated with numerous genes and pathways. New transformation capabilities to design and edit multiple genes within a plant genome more efficiently and cost-effectively are needed, particularly for nonfood crops intended as feedstocks for a broader bioeconomy. This capability is intended to increase current capacity for bioenergy crop genomic transformation through research to identify barriers in crop transformation and develop breakthroughs to overcome such barriers by leveraging existing capabilities at Office of Science user facilities. More cost-efficient transformation methods will democratize these techniques across the scientific community allowing accelerated exploration of plant genomic engineering for a variety of clean energy, carbon management, and bioproduct production purposes.

Potential to Contribute to World-Leading Science in the Next Decade

A *Absolutely central*

B Important

C Lower priority

D Don't know enough yet

Readiness for Construction

A *Ready to initiate construction*

B Significant scientific/engineering challenges to resolve before initiating construction

C Mission and technical requirements not yet fully defined

Overall Assessment

The BERAC subcommittee finds that the establishment of this PTC is timely and highly desirable. The PTC will be a unique facility that meets a central need in plant sciences. Precision genome editing technologies such as CRISPR offer a heretofore unimagined ability to modify any plant genome in a highly targeted and societally acceptable manner and promise to revolutionize plant-based food, feed, and fuel production. BER recently organized a workshop “Overcoming Barriers in Plant Transformation: A Focus on Bioenergy Crops” and concluded that “in the next five to ten years, transformation demand is expected to increase at least twentyfold, and more sophisticated genomic engineering will require efficiency increases of at least one order of magnitude” (U.S. DOE 2024). The subcommittee’s overall recommendation is that the establishment of the PTC is given the highest level of priority.

Scientific Importance

The subcommittee places the PTC in the category of (A) absolutely central. Given the essentiality of plant transformation, both for improving understanding of

fundamental plant biology and for agricultural applications, coupled with the huge unmet current demand for plant transformation capacity across the plant sciences, there is no question that such a DOE facility would “contribute to world-leading science in the next decade.” Currently, there is no existing large-scale facility that addresses the challenges of facile transformation of diverse plant species. In this context, the recent recognition by the National Science Foundation and U.S. Department of Agriculture of the centrality of plant transformation provides assurance that the PTC will address needs of the broad plant science community.

Construction Readiness

The subcommittee places the PTC in the category (A) ready to initiate. Organization and priorities for the PTC have been defined in a recent workshop (U.S. DOE 2024). The subcommittee notes that the mission need is clear, and the knowledge trust is available to immediately establish the PTC at one or more DOE facilities to better serve the bioenergy community and address plant transformation challenges during the Critical Decision process.

Bioeconomy Accelerator Facility

Construction Project • Total Project Cost Range: To be determined

Project Description

Construction of the Bioeconomy Accelerator Facility (BAF) either as a stand-alone Office of Science user facility or as part of an existing Office of Science user facility would speed the transition of foundational scientific discoveries and advance the U.S. bioeconomy. The facility would address the basic science bottlenecks that preclude a broader ability to scale engineered biological processes toward higher volumes, titers, and yields and to move from bench scale to pre-commercial scale for microbial (aerobic/anaerobic bacteria, viruses, fungi) growth and fermentation. The capability would rely on partnerships to make use of capabilities and resources available through the Joint Genome Institute, National Microbiome Data Collaborative, and Microbial Molecular Phenotyping Capability at the Environmental Molecular Sciences Laboratory. Currently, there are very few mid-scale testbeds to mid-commercial-scale production facilities [e.g., Advanced Biofuels and Bioproducts Process Development Unit (ABPDU) supported by the DOE Bioenergy Technologies Office (BETO)], but the difficulty with these is that they are only available on an op-ex basis, meaning ABPDU collaborators pay for personnel time and materials access and ABPDU staff then only work on that project. This capability would be open to scientific users.

The BAF would be part of an overall pipeline from foundational research supported by BER to proof of concept, thereby transitioning more easily to either a BETO-funded entity (i.e., an ABPDU) or to a commercial/industrial partner. The BAF would enable scientists to design microbial or plant systems for scale-up of chemicals and products produced from renewable resources that displace petroleum (e.g., bioplastics and biomaterials) that are relevant to accelerating a broader U.S. bioeconomy and advance the energy, economic, and national security of the United States.

Potential to Contribute to World-Leading Science in the Next Decade

- A Absolutely central
- B Important**
- C Lower priority
- D Don't know enough yet

Readiness for Construction

- A Ready to initiate construction
- B Significant scientific/engineering challenges to resolve before initiating construction
- C Mission and technical requirements not yet fully defined**

Overall Assessment

The BAF is important and could contribute to world-leading science because of its potential to increase the availability of domestic scale-up facilities, expand capabilities for scale-up to nonstandard processes, and couple scale-up research with research on upstream and downstream processing. This potential is largely unready to be realized because of the lack of a clear mission and set of objectives that would distinguish the BAF from other existing facilities.

Scientific Importance

There is significant enthusiasm from stakeholders for more facilities to enable researchers to scale up laboratory pilot-scale reactors to proof of concept. Both stakeholders and several recent reports indicate a deficit in U.S. scale-up facilities. Additionally, many existing facilities cannot easily meet emerging needs, including those that utilize nonmodel microorganisms, employ substrates beyond simple carbohydrates, or require reactors other than a stirred-tank reactor. Stakeholders are also interested in whether the BAF could couple scale-up research with upstream and downstream processes, such as feedstock deconstruction, strain engineering, or downstream processing and separations.

While enthusiasm for new capabilities is high and some potential research areas have been identified, a significant challenge is that several facilities that purport to address part of the mission of the proposed BAF already exist and are seeking to expand. Whether such expanded facilities would have both the technical capabilities and accessibility to meet the needs of the BER community remains unclear. Thus, BER may need to develop a BAF, but currently, the BAF lacks a clear mission and unique objectives distinguishable from existing facilities.

Construction Readiness

Several mission and technical requirements would need to be defined before a BAF could be deemed ready to initiate construction. Mission requirements need to be clarified by identifying two sets of basic science knowledge gaps: (1) gaps that currently preclude predictive scale-up of engineered biological processes from 1-L benchtop reactors to hundreds of liters and (2) gaps around coupling scale-up to upstream and/or downstream processes. These must be distinguishable from development and engineering needs at this scale for the BAF to remain within BER's focus on basic research. A second requirement that must be defined is the degree to which the BAF would integrate strain engineering and upstream or downstream processing with scale-up research; including these efforts alongside scale-up research would lead to a facility with significantly different technical requirements than one focused only on scale-up research. Third, the data-sharing requirements of the BAF must be defined. While aggregating data from multiple sources will critically advance a generalized science of scale-up, such data-sharing requirements may be unviable for industrial users. Addressing these key points will be critical to ensure BAF's mission, central objectives, and uniqueness from existing facilities are defined before its launch.

Recommendation

Given enthusiasm for BER investment in the BAF, the subcommittee recommends (1) clearly defining the contributions for such a facility by BETO and BER, and (2) convening a workshop to define the scientific needs for such a facility.

Earth System Modeling and Analysis Center User Facility

Construction Project • Total Project Cost Range: To be determined

Project Description

This project entails development of an Earth system modeling and analysis center, including computational hardware, new software, visualization tools, and user interfaces. A BER Earth System Modeling and Analysis Center (ESMAC) User Facility will address scientific gaps, enhance progress toward BER Grand Challenges in Earth and Environmental Systems Sciences, and address a BERAC recommendation by developing a computational user facility for rapid design, generation, evaluation, and diagnosis of Earth system model simulations, as well as analysis of ensemble predictions and data-model synthesis. The user facility will bring together theory, models, observations, and computation to accelerate fundamental research into the complex biological, ecological, and hydrological processes in Earth system science and the interactions between natural and human systems, spanning a large range of temporal and spatial scales. As noted in the *Scientific User Research Facilities and Biological and Environmental* report (BERAC 2018), due to increasing software, model, and computational complexity, it is extremely difficult for users outside the model development community to run state-of-the-art Earth system models such as the Energy Exascale Earth System Model (E3SM).

The ESMAC User Facility would integrate and leverage BER's unique capabilities in modeling, simulation, multiscale analysis, and data management, spanning small scales involving ecosystems and communities to global scales. With dedicated computational, data analysis, and visualization resources and staffed by scientists with Earth system model expertise, ESMAC would enable a new level of investigation through simulation and analysis to improve understanding of the Earth system, inform planning for climate change mitigation and adaptation, assess impacts on built infrastructure, and test a wide range of energy production, carbon management, and climate security scenarios. ESMAC will be a BER community resource for modeling, hypothesis testing, data synthesis, data analytics, and visualization. The facility would further develop BER's E3SM and its modules into a community resource available to the scientific community to conduct their own simulations and model experiments.

Potential to Contribute to World-Leading Science in the Next Decade

A *Absolutely central*

B Important

C Lower priority

D Don't know enough yet

Readiness for Construction

A Ready to initiate construction

B *Significant scientific/engineering challenges to resolve before initiating construction*

C Mission and technical requirements not yet fully defined

The facility could also support the development and execution of community-requested large ensemble simulations that are too computationally expensive for single investigators to conduct. The model would be coupled with advanced observational metrics for model benchmarking. User facility staff would work with users to design and execute specific model simulations for hypothesis testing, digital twinning of the Earth system, future climate scenarios, and other applications in support of DOE's broader mission involving energy and economic security. The facility would develop and make available software tools and user interfaces for advanced data analysis, data assimilation, artificial intelligence and machine learning, model evaluation, and visualization. The need for an Earth system modeling and analysis center has been highlighted in the *Grand Challenges for Biological and Environmental Research* report (BERAC 2017) and the BERAC scientific user facility report (BERAC 2018).

Overall Assessment

ESMAC is absolutely central in its potential to contribute to world-leading science. The DOE E3SM is a world-leading model in its class, both scientifically and computationally, and would serve as the foundation of ESMAC. User facilities similar to ESMAC are in place elsewhere: Europe, Japan, and, in the United States, at the National Science Foundation's (NSF) National Center for Atmospheric Research (NCAR). However, ESMAC would be unique in that its foci would include human interactions with the Earth system and biological interactions with physical and chemical components of the Earth system. E3SM also uniquely places strong application emphasis on the nation's energy sector. A primary purpose of ESMAC would be to expand engagement with a larger community of scientists beyond the researchers at DOE national laboratories where E3SM development is currently centralized. This effort would increase analysis by external research communities and build collaborative opportunities between these groups and E3SM developers at national labs.

Scientific Importance

Dedicated computing and analysis at DOE Advanced Scientific Computing Research (ASCR) facilities, which are envisioned to undergo transformative enhancement in response to this charge, should be explored. Discussions with ASCR colleagues responding to this charge indicate interest in pursuing this. An

important element of integrating ASCR and ESMAC facilities would be exploiting new, emergent synergies between computational science, hardware and software design, and Earth system modeling from the earliest stages. That is, the subcommittee envisions not just computational machinery and support staff through the ASCR relationship, but substantial scientific collaboration, all the more essential given the vast range of directions scientific computing may take in the next decade (e.g., diverse hardware and software developments, artificial intelligence and machine learning, and quantum computing).

Construction Readiness

The subcommittee finds that significant scientific and engineering challenges need to be resolved before initiating construction. The proposal requires further elaboration, especially regarding whether it would provide dedicated computing—perhaps as part of ASCR program facilities—or function in a more limited way. NSF provides both dedicated computing and community engagement through NCAR for its Community Earth System Model. The subcommittee recommends exploring how ESMAC can complement Earth system modeling activities at NSF as well as other agencies and internationally. More detailed scoping for ESMAC should be developed through community workshops, which would address the scientific and engineering challenges and how ESMAC will complement the other national and international activities noted above.

EcoPODs and Smart Soil Systems

Major Item of Equipment • Total Project Cost Range: To be determined

Project Description

This project involves laboratory test chambers (EcoPODs) for integrated plant-microbe-soil experiments to test hypotheses of ecosystem function under controlled environmental conditions as well as new types of sensors (Smart Soil Systems) for physical, chemical, and biological characterization of natural systems.

BER's programs seek to gain a predictive understanding of complex biological and environmental processes across a range of observational scales. The research is inherently multidisciplinary and complicated due to the 3D spatial and temporal dynamics that govern natural processes. There is a need to conduct experiments under controlled laboratory conditions to identify key variables impacting the functioning of ecosystems and compare results to conditions and studies conducted at field sites that are monitored using advanced sensing capabilities.

Fully instrumented laboratory test chambers are where intact soil systems containing plants, associated microbiomes, and soil structures can be measured and manipulated in the laboratory while controlling key environmental variables. The chambers enable an extensive battery of measurement capabilities not possible or not allowed (e.g., isotopic methods) in the environment. Comparison of chamber results with measurements in the environment using advanced sensors developed using the Smart Soil Systems allows laboratory-to-field iteration (and vice versa) to converge on gaining a predictive understanding of ecosystem function. EcoPODs and Smart Soil Systems afford the ability to isolate intact plant-microbe-soil blocks from the environment to conduct "twinning" laboratory and field research. The test chambers enable detailed analysis, characterization, and experimentation under controlled conditions in the laboratory that cannot be controlled in the field. These fully enclosed systems allow a full range of gaseous, solid, liquid, and biological sampling under multiple spatial, temporal, and statistical experimental designs.

The capabilities, when paired with iterative research and monitoring using advanced sensors at twinned field sites, represent cutting-edge approaches to gain whole ecosystem functioning for a variety of BER climate and environmental missions. The test chambers will be deployed in the new Lawrence Berkeley National Laboratory Biological and Environmental Program Integration Center (BioEPIC) building, home to several BER Scientific Focus Area research projects from across both BER divisions

Potential to Contribute to World-Leading Science in the Next Decade

A Absolutely central

B Important

C *Lower priority*

D Don't know enough yet

Readiness for Construction

A Ready to initiate construction

B *Significant scientific/engineering challenges to resolve before initiating construction*

C Mission and technical requirements not yet fully defined

engaged in environmental research. The equipment will enable researchers to bridge gaps in translating smaller-scale plant–microbe–soil processes to larger-scale ecosystem processes that span the BER portfolio. A particular focus would be to merge genome-enabled mechanistic models of microbial and plant metabolism with biogeochemical models to gain a more spatiotemporal understanding of biological impacts on environmental processes.

Scientific Importance

The subcommittee has concerns about the EcoPODs and Smart Soil Systems' (EcoPASSS) uniqueness, its utility to the broad BER community, and its value in informing processes in the field. A major concern is that the proposed equipment is not novel; there are other facilities with similar capabilities. While EcoPASSS would be an important resource for the BioEPIC research group, it is less clear how central the equipment would be to the larger BER community. Lastly, a major goal of EcoPASSS is to bridge laboratory experiments and ecosystem measurements to better understand the impacts of soil–plant–microbe interactions. This goal is perceived as unrealistic in the absence of a stronger link to field studies (e.g., Bioenergy Research Centers or the Environmental Molecular Sciences Laboratory) and incorporation of scaling to realistic agroecosystem modeling.

Construction Readiness

While this equipment could be purchased immediately, the subcommittee is concerned that the currently proposed configuration lacks the flexibility that would position EcoPASSS to have a community-wide scientific impact in the 10-year timeframe. The fabricated ecosystem effort has been ongoing since 2017 with workshops in 2018 and 2020. An existing set of pilot equipment exists and has been tested, although the subcommittee is unaware of any publications or reports resulting from this work. If this system is adopted, EcoPOD units could be purchased immediately. Space is available in the new BioEPIC building to house the new equipment. However, it would be valuable to consider other systems with more interchangeability and expandability or connection to existing U.S. phytotrons or growth facility infrastructure. Without this connectivity and expandability, there is concern this investment will not be able to push scientific frontiers over an extended time horizon.

Visual Proteomics Capability

Major Item of Equipment • Total Project Cost Range: To be determined

Project Description

A Major Item of Equipment (MIE) is needed to enable visual proteomics within microbial cells. With a visual proteomics capability, scientists would be able to visualize individual proteins as well as their dynamics and interactions with other molecular constituents in cells. These interactions lead to the creation of biological assemblies, including a variety of different types of macromolecular machines.

Initial efforts would focus on investigations of microbial cells, although the capability could potentially be used for plant cells. The basis for this capability would be a mass spectrometry system. The Visual Proteomics MIE would be to design, build, and initiate operations of a mass spectrometry-based capability within an Office of Science user facility that would be made available to users and would be capable of enabling users to visualize proteins and their dynamics within the cellular matrix for a variety of microbes. A visual proteomics capability would not only enable users to visualize the proteome of a microbe but would enable them to quantify proteins within the cellular matrix and to study the dynamics of protein–protein interactions and other metabolic activities in real time within a given cell.

The understanding enabled by this capability could be used to determine the potential for modifying the dynamics and quantity of proteins and other cellular components within cells and communities to address BER and DOE needs. A visual proteomics capability would allow detailed investigation and visualization of gene expression processes within a wide variety of plant and microbial cells. This MIE would provide the capabilities needed to more fully understand protein expression, structural formation, localized activity, and the full cycle of protein structures in cells. The capability has applications in fundamental biological proteomics and biosystems design research.

Potential to Contribute to World-Leading Science in the Next Decade

- A Absolutely central
- B Important
- C Lower priority

D *Don't know enough yet*

Readiness for Construction

- A Ready to initiate construction
- B *Significant scientific/engineering challenges to resolve before initiating construction*
- C Mission and technical requirements not yet fully defined

Overall Assessment

The subcommittee concludes that it is too early to start building a Visual Proteomics Capability (VPC). Once research studies define the scope of such a capability, a VPC can be better planned. If successful, a well-designed VPC would open many new directions in microbial cell biology and metabolism research, but it is not available as a turnkey system.

Scientific Importance

The concept of spatial or visual proteomics aims to systematically identify the complete protein composition of a cell or its subcellular regions, mapping how protein composition varies spatially within or between cells. This ambitious endeavor seeks to delve deeper than traditional bulk sample proteomics, using mass spectrometry (MS) methods to precisely measure peptide masses derived from proteins and correlate these to genomic predictions. However, MS techniques encounter sensitivity challenges, especially in detecting and quantifying proteins in minuscule quantities, such as those found in single cells. The proposed method aims to enhance this capability through spatially resolved MS analyses within individual cellular regions.

Historically, two primary approaches have been employed for spatial proteomics. The first involves tagging genes with fluorescent markers then using light microscopy to visualize protein distribution within the cell. Although widely used in research, especially in yeast and mammalian cells, this method demands significant automation and is organism-specific, limiting its broader applicability. The second method involves creating extensive collections of antibodies for high-throughput immunofluorescence imaging. This technique offers high spatial precision without genetic modification but requires substantial financial investment and is similarly limited by its species-specific nature.

Alternative methods applicable to a broader range of organisms include organelle fractionation and cryo-electron microscopy (cryo-EM). Organelle fractionation separates cellular components for

MS analysis, but it lacks the spatial specificity to observe intracellular protein distribution variations. Cryo-EM, termed visual proteomics, freezes cells for ultra-high-resolution imaging, identifying proteins through their 3D structures—a method now enhanced by computational predictions from tools like AlphaFold. However, cryo-EM's high cost and limited imaging volume restrict its use for large cells or comprehensive cellular mapping.

The proposed innovative scanning MS technique addresses these limitations by using a laser scanner to target and release peptides from specific subcellular areas for MS analysis. This method, which has shown promise in differentiating lipid compositions among cell populations, represents a significant advancement in spatial proteomics. It not only overcomes sensitivity issues but also offers a spatially resolved analysis within single cells, potentially transforming understanding of cellular complexity and the intricate dynamics of protein distribution and function at the microscopic level.

Regarding the first charge question of importance, the subcommittee places the VPC in the category of (D) don't know enough yet. The concept of spatial proteomics is relatively new, and it has mostly been employed in a few well-established model systems. What scientists will learn when it is applied to a broader range of organisms including plants, algae, and bacteria is still an open question. Identifying central questions that can best be answered by this type of technique thus remains an important goal to determine what such a VPC will look like.

Construction Readiness

The subcommittee places the VPC in the category of (B) significant scientific/engineering challenges to resolve before initiating construction. Scanning MS methods like Scanning MALDI-MSI are already used for proteomics and lipidomics in tissues where data can be obtained from individual cells among a group of cells. The main factor limiting the current resolution of MS-based spatial proteomics is not the resolution of the scanning itself but the quantity of peptides that can be released from a very small sample. MS-based

proteomics has become more sensitive and reached the point that protein from a single cell can be analyzed in some cases. But the current proposal addresses a much smaller spatial scale, seeking to obtain proteome data from different subregions within a single cell, which could itself be as small as a bacterium. This appears to be beyond the capabilities of current instrumentation and would therefore require a substantial research effort to increase sensitivity.

Phased Array Radar

Major Item of Equipment • Total Project Cost Range: To be determined

Project Description

This project involves a next-generation phased array radar for atmospheric research to upgrade current radars in use as part of the Atmospheric Radiation Measurement (ARM) user facility. Estimated cost varies depending on wavelength, array size, and polarization capabilities. A next-generation scanning radar system for the ARM user facility is and will be needed to maintain state-of-the-science capabilities within ARM. Traditional scanning radar systems mechanically rotate and tilt the radar dish to sample different parts of the atmosphere. In a phased array radar, the antenna is a flat panel that remains stationary. The antenna is composed of a grid of elements that each transmit and receive signals, and the radar beam is steered electronically instead of mechanically through phase shifting of the signals.

The advantage of phased array radars is much faster directional sampling (without the limitations of mechanical inertia of conventional radars), fewer mechanical parts, and potentially more robust systems (as single antenna elements can fail without failure of the entire system). Phased array radars can complete a 90-degree sector scan of the atmosphere approximately four to five times more quickly than conventional radars, allowing more rapid sampling of cloud and precipitation systems and cloud tracking. Electronic antenna steering also allows advanced adaptive scanning and edge computing techniques. Additionally, future observational modes can be implemented via software updates rather than hardware changes. A phased array radar system will allow autonomous adaptive sampling of cloud and precipitation systems. The enhanced temporal resolution and antenna steering will allow quasi-continuous observation and Lagrangian tracking of cloud systems, enabling analyses of precipitation formation, convective updrafts and downdrafts, and cloud dynamics to improve representation of these processes in DOE Earth system models. Upgrading the radar systems currently deployed as part of the ARM portfolio will greatly enhance capabilities to analyze atmospheric phenomena more efficiently and at smaller time intervals.

Potential to Contribute to World-Leading Science in the Next Decade

- A** *Absolutely central*
- B** Important
- C** Lower priority
- D** Don't know enough yet

Readiness for Construction

- A** *Ready to initiate construction*
- B** Significant scientific/engineering challenges to resolve before initiating construction
- C** Mission and technical requirements not yet fully defined

Overall Assessment

The phased array radar (PAR) is absolutely central and ready to initiate construction. The more rapid scanning will transform the observational basis for understanding cloud dynamics and microphysics. The technology is quite well developed. The National Science Foundation (NSF) is in the process of implementing PAR on aircraft, and PAR is being considered to replace the National Oceanic and Atmospheric Administration (NOAA) National Weather Service operational Doppler warning radar network. The imperative for PAR was highlighted in the 2017 BERAC Grand Challenges report (BERAC 2017).

Scientific Importance

Upgrading DOE's ARM ground-based research radar is absolutely central to maintaining DOE's world-leading suite of field observational capabilities. The DOE ARM PAR facility would be unique in providing ground-based observations for research studies of cloud systems, which are especially important to understanding rapidly evolving convective storms.

This understanding is essential not only for weather applications but also to improve representation of convection in advanced Earth system models.

Construction Readiness

PAR's status as (A) ready to initiate construction has been established through previous NSF and NOAA applications. The subcommittee recommends strongly that the PAR facility maximize its capabilities regarding wavelength choices, polarization, and other recent technological developments. The massive increase in temporal and spatial detail PAR would provide would impart opportunities to interpret PAR observations using next-generation cloud chambers, which have been proposed to include all water phases and turbulence. The subcommittee's endorsement of PAR's scientific potential and construction readiness is strong regardless of the status of the cloud chamber (see p. 4) also under consideration in this charge. The subcommittee notes unprecedented opportunities for synergy between laboratory and field studies should both facilities be constructed.

Appendix A

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Appendix B

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Acronyms and Abbreviations

3D	three-dimensional	DRACO	Drizzle, Aerosol, and Cloud Observation chamber
ABPDU	Advanced Biofuels and Bioproducts Process Development Unit	E3SM	Energy Exascale Earth System Model
ACO	Aerosol and Cloud Observation chamber	EcoPASSS	EcoPODs and Smart Soil Systems
ARM	Atmospheric Radiation Measurement user facility	ESMAC	Earth System Modeling and Analysis Center
ASCR	DOE Advanced Scientific Computing Research program	FY	fiscal year
BAF	Bioeconomy Accelerator Facility	M2PC	Microbial Molecular Phenotyping Capability
BDC	BER Data Center	MIE	Major Item of Equipment
BER	Biological and Environmental Research program	MS	mass spectrometry
BERAC	BER Advisory Committee	NCAR	National Center for Atmospheric Research
BETO	DOE Bioenergy Technologies Office	NOAA	National Oceanic and Atmospheric Administration
BioEPIC	Biological and Environmental Program Integration Center	NSF	National Science Foundation
CD	Critical Decision	PAR	Phased Array Radar
cryo-EM	cryo-electron microscopy	PTC	Plant Transformation Capability
DOE	U.S. Department of Energy	VPC	Visual Proteomics Capability