

## 2023 Biological and Environmental Research Facilities Charge

In response to Dr. Berhe's December 2023 Facilities Charge, the Office of Science (SC) Biological and Environmental Research (BER) is providing the following list of projects for consideration by the subcommittee.

### ***Category: Construction Projects***

#### **Microbial Molecular Phenotyping Capability (M2PC)**

*Total Project Cost (TPC) range: \$100 - 167M*

M2PC will provide unique automated and high-throughput capabilities within a current BER user facility (EMSL) to phenotype vast numbers of microbial isolates providing crucial functional data on microbial communities from a wide variety of environments. This facility upgrade achieved CD-0 in FY 2021. The M2PC project will design and construct a new capability that will provide a range of wet chemistry and instrumentation space conducive for highly autonomous operations, as part of an SC 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 are 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 BERAC 2017 Grand Challenges report.

#### **Drizzle, Aerosol, and Cloud Observation (DRACO) Chamber**

*Total Project Cost (TPC) range: \$34 - 47M*

The DRACO Chamber is an experimental facility for controlled testing of cloud and aerosol processes. This facility upgrade achieved 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 10m 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, increased 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 BERAC 2022 International Benchmarking report and the BERAC 2018 Scientific User Facilities report.

## **BER Data Center**

*Total Project Cost (TPC) range: TBD*

A centralized data and mid-range computational infrastructure to tackle the challenges of exponential growth in data volumes due to improvements in instrument resolution and laboratory automation, model complexity, and increases in the rate of data generation within BER's Biological, Earth, and Environmental research programs. BER's focus on systems science leads to the creation of data that spans from molecular to global spatial scales, nanoseconds to decadal temporal scales, and across 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, and metadata. A BER Data facility will promote harmonization of data management and analysis services (including the use of AI and ML 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 multi-disciplinary research efforts across BER. The need for this capability was highlighted in the BERAC 2018 Scientific User Facilities report.

## **Plant Transformation Capability**

*Total Project Cost (TPC) range: TBD*

The Plant Transformation Capability (PTC) is intended to become a new capability to be added to an existing user facility (i.e., JGI) 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 it 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 non-food 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 SC 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.

### **Bioeconomy Accelerator Facility**

*Total Project Cost (TPC) range: TBD*

Construction of the Bioeconomy Accelerator Facility (BAF) either as a stand-alone SC User Facility or as part of an existing SC 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 towards 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 Joint Genome Institute, National Microbiome Data Collaborative, and M2PC at 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 DOE Biotechnologies Technology 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 (ex. bioplastics, biomaterials, etc.) that are relevant to accelerating a broader U.S. bioeconomy and advance the energy, economic, and national security of the U.S.

### **Earth System Modeling and Analysis Center, User Facility**

*Total Project Cost (TPC) range: TBD*

Development of an earth system modeling and analysis center, including computational hardware and development of new software, visualization tools, and user interfaces. A BER Earth System Modeling and Analysis Center (ESMAC) User Facility will address scientific gaps, enhance progress towards BER Grand Challenges in Earth and Environmental System 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 BERAC 2018 User Facilities Report, 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, multi-scale analysis, and data management, spanning small scales involving ecosystems and communities to the 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 Energy Exascale Earth System Model (E3SM) and its modules into a community resource, available to the scientific community to conduct their own simulations and model experiments. 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/machine learning, model evaluation, and visualization. The need for a Earth system modeling and analysis center has been highlighted in the BERAC 2017 Grand Challenges report and the BERAC 2018 Scientific User Facility report.

### ***Category: Major Item of Equipment (MIE)***

#### **MIE – EcoPODs and Smart Soil Systems (EcoPaSSS)**

*Total Project Cost (TPC) range: TBD*

Laboratory test chambers (EcoPODs) for integrated plant-microbe-soil experiments to test hypotheses of ecosystem function under controlled environmental conditions, and 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 multi-disciplinary 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 allow for an extensive battery of measurement capabilities not possible (or not allowed ex. isotopic methods) in the environment. Comparison of chamber results with measurements in the environment using advanced sensors developed using the Smart Soil Systems allows lab-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 "twinned" laboratory and field research. The test chambers allow 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 BioEPIC building, home to several BER Scientific Focus Area (SFA) research projects from across both BER divisions 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 seek to merge genome-enabled mechanistic models of microbial and plant metabolism with biogeochemical models to gain a more spatio-temporal understanding of biological impacts on environmental processes.

### **MIE – Visual Proteomics Capability**

*Total Project Cost (TPC) range: TBD*

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 on 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 SC 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 with cells and communities to address BER/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. The MIE would provide the capabilities needed to more fully understand protein expression, structural formation, localized activity and full cycle of protein structures in cells. The capability has applications in fundamental biological proteomics and biosystems design research.

### **MIE - Phased Array Radar**

*Total Project Cost (TPC) range: TBD*

A next generation phased array radar for atmospheric research to upgrade current radars in use as part of the ARM program. 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/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 4-5 times more quickly than conventional radars, allowing more rapid sampling of cloud/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/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.