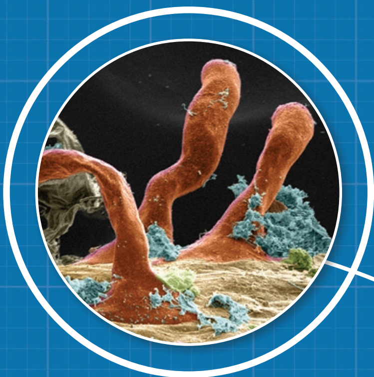
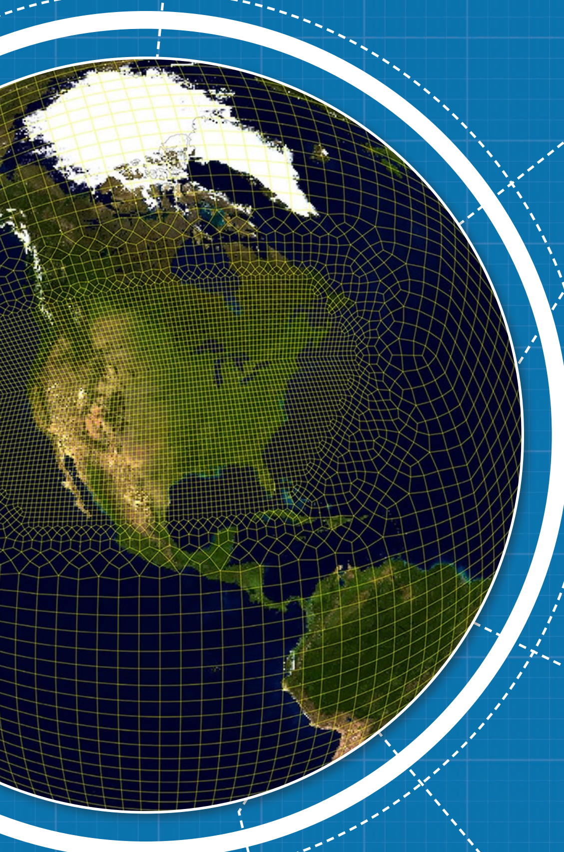
DOE/SC-0208

U.S. SCIENTIFIC LEADERSHIP

Addressing Energy, Ecosystems, Climate, and Sustainable Prosperity





Report from the BERAC Subcommittee on International Benchmarking

U.S. Scientific Leadership

Addressing Energy, Ecosystems, Climate, and Sustainable Prosperity

Report from the BERAC Subcommittee on International Benchmarking

Subcommittee Co-Chairs

Maureen McCann
National Renewable Energy Laboratory

Patrick Reed
Cornell University

Designated Federal Officer

Tristram West
U.S. Department of Energy
Biological and Environmental Research Program

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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U.S. Scientific Leadership

Addressing Energy, Ecosystems, Climate, and Sustainable Prosperity

Report from the BERAC Subcommittee on International Benchmarking

December 2022

U.S. DEPARTMENT OF ENERGY | Office of Science

Biological and Environmental Research Program

Charge Letter

Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 8, 2020

Dr. Bruce Hungate
Regents' Professor, Biological Sciences
Northern Arizona University
SLF Building 17, Room 300A
600 South Knoles Dr.
Flagstaff, Arizona 86011

Dear Dr. Hungate:

I sincerely appreciate the work that the Biological and Environmental Research Advisory Committee (BERAC) and the Committee of Visitors recently completed on the review of the Earth and Environmental Systems Sciences Division management processes. I am also grateful for the continued service that BERAC has provided despite the challenges of the COVID-19 situation. Please know that the Office of Science and the Department of Energy value the important work of BERAC.

I am writing because I would like BERAC to consider the Office of Biological and Environmental Research's (BER) international leadership in the research community and whether there are opportunities or pathways available to increase this leadership. Recent completion of the BERAC reports on Grand Research Challenges in 2017 and on Scientific User Facilities in 2018 have helped to identify future paths of research for BER. Understanding the future research needs and how user facilities may respond to those needs is an important component of maintaining scientific excellence. Another important component is leadership in the international arena. This is particularly important in a time with changing technologies, changing economies, and changing environmental threats and conditions.

Therefore, I would like BERAC to consider strategies to increase BER's international research competitiveness. These strategies will strengthen BER's ability to conduct world-class science in research areas that have been previously identified in the Grand Challenges report. I ask BERAC to consider the following questions when considering useful and appropriate strategies that might be included in an implementation plan:

- Within the BER-supported topical research areas and facility capabilities, in which areas and capabilities, presently or in the foreseeable future, does BER lead in the international community, and in which areas does leadership require strengthening? In identifying these areas, please consider their critical mission relevance, recent history, the status quo, observable trends, and evidence-based projections.
- Are there key international partnerships that could strengthen BER science output and increase global visibility of BER?

- To preserve and foster U.S. leadership with resource constraints, is there a preferred optimization for organizing research, collaboration, and funding mechanisms among labs, universities, and other federal agencies? Are there other key efficiencies and balances that should be considered and modified to improve U.S. leadership in BER research areas?
- For someone deciding whether to pursue a scientific career, or a mature scientist considering whether to stay in the U.S., how can BER programs and facilities be structured and managed to create incentives that will attract and retain talented people? What are the key opportunities for BER in attracting and enhancing careers in BER-supported science?

In general, this study will serve as a benchmark for BER's international standing in core research areas within the BER research portfolio. Existing core areas are represented in the Grand Challenges report and by the BER Science Focus Areas. This study should consider any programmatic or management areas that may be modified in order to increase BER's international standing in the core areas, and these should be presented as specific strategies that DOE Office of Science could implement and track. Results of this study should be reported out at the Spring BERAC meeting in 2022.

Thank you again for your service and that of the committee. I hope that you and yours remain safe and healthy in this challenging time.

Sincerely,

Chris Fall
Director
Office of Science

cc. Sharlene Weatherwax

Subcommittee Members

Co-Chairs

Maureen McCann, *National Renewable Energy Laboratory*

Patrick Reed, *Cornell University*

Designated Federal Officer

Tristram West, *U.S. Department of Energy Biological and Environmental Research Program*

Working Group Co-Leads

Crysten Blaby, *Lawrence Berkeley National Laboratory*

Brian H. Davison, *Oak Ridge National Laboratory*

Robert F. Fischetti, *Argonne National Laboratory*

Ann M. Fridlind, *NASA Goddard Institute for Space Studies*

Michael N. Gooseff, *University of Colorado–Boulder*

Kerstin Kleese van Dam, *Brookhaven National Laboratory*

Himadri Pakrasi, *Washington University in St. Louis*

Kristala Prather, *Massachusetts Institute of Technology*

Margaret S. Torn, *Lawrence Berkeley National Laboratory*

John Weyant, *Stanford University*

Shaocheng Xie, *Lawrence Livermore National Laboratory*

Huimin Zhao, *University of Illinois at Urbana-Champaign*

Working Group Members

Ana Alonso, *University of North Texas*

Ludmilla Aristilde, *Northwestern University*

Allison A. Campbell, *emerita Pacific Northwest National Laboratory*

Kenneth James Davis, *The Pennsylvania State University*

Ben Evans, *Australian National University*

Efi Foufoula-Georgiou, *University of California–Irvine*

Serita Frey, *University of New Hampshire*

Ramon Gonzalez, *University of South Florida*

Nathan Hillson, *Lawrence Berkeley National Laboratory*

Janet Jansson, *Pacific Northwest National Laboratory*

Klaus Keller, *Dartmouth College*

Markus Kleber, *Oregon State University*

Costas Maranas, *The Pennsylvania State University*

Gerald A. Meehl, *National Center for Atmospheric Research*

Jennifer Pett-Ridge, *Lawrence Livermore National Laboratory*

Johannes Quaas, *Leipzig University*

Seung Yon (Sue) Rhee, *Carnegie Institution for Science*

G. Philip Robertson, *Michigan State University*

Alistair Rogers, *Brookhaven National Laboratory*

Tim Scheibe, *Pacific Northwest National Laboratory*

Thomas R. Schneider, *European Molecular Biology Laboratory*

Gary Stacey, *University of Missouri*

Detlef van Vuuren, *Utrecht University and PBL Netherlands Environmental Assessment Agency*

Stan Wullschleger, *Oak Ridge National Laboratory*

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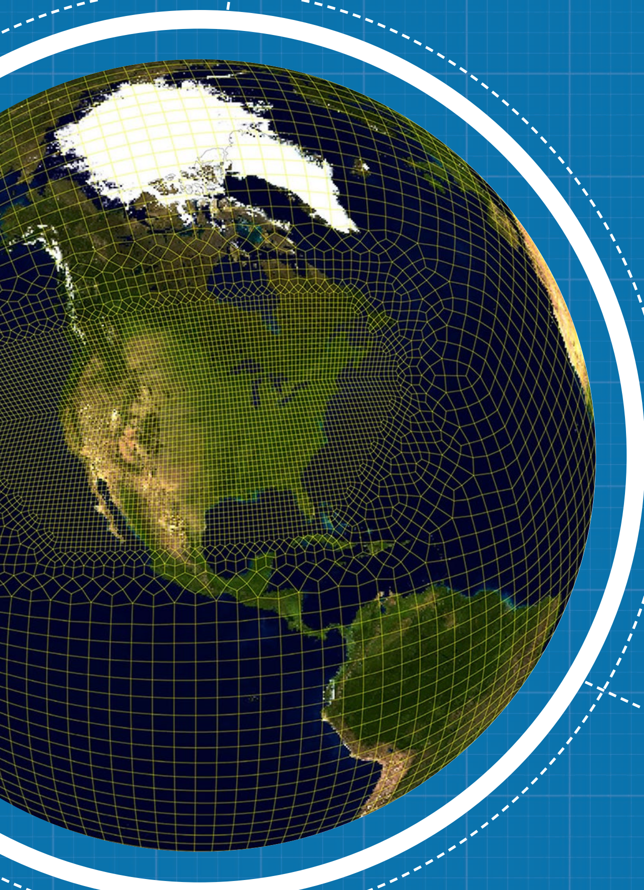
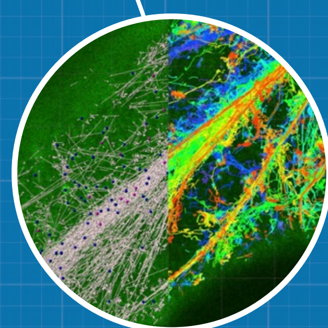
Executive Summary





Subcommittee Co-Chairs

Maureen McCann, *National Renewable Energy Laboratory*
Patrick Reed, *Cornell University*

Additional Contributor

Efi Foufoula-Georgiou, *University of California–Irvine*

Executive Summary

The research mission of the U.S. Department of Energy's (DOE) Biological and Environmental Research (BER) program is to support transformative science and scientific user facilities to achieve a predictive understanding of complex biological, Earth, and environmental systems for clean energy and climate innovation. BER mission areas are strategically situated at the nexus of critical global challenges in climate change, energy transitions, and sustainable prosperity. The program's investment portfolio supports and sustains "Big Science" to advance frontiers in genome-enabled biology and the interdependencies of physical and biogeochemical Earth system processes. BER's world-leading facilities enable major scientific discoveries across a global network of supported researchers. Unique in scale and scope, the program's mission areas range from molecular and genomic biosciences to the global dynamics of the atmosphere, oceans, and continents, with a common thread of life across environments.

In fiscal year 2021, BER's $753 million budget supported 1,510 PhD scientists and 530 graduate students at more than 140 academic and nonprofit organizations and at 12 DOE national laboratories. Its facilities supported more than 3,900 users globally. BER's research investments and its experimental, observational, and computational user facilities have played central roles in (1) Nobel Prize–winning science, (2) major innovations in sustainable bioenergy, (3) world-leading ecosystem-scale experiments, (4) key global efforts addressing climate change, and (5) recent therapeutic discoveries in the fight against COVID-19. These achievements illustrate BER's unique position in the federal funding landscape as a driver of transformative and use-inspired discovery science.

Assessing BER's International Standing

Beginning in 2019, the director of the DOE Office of Science began issuing first-of-a-kind charges to the federal advisory committees of several Office of Science programs, asking them to benchmark the programs' international research competitiveness. The Basic Energy Sciences Advisory Committee (BESAC) received the charge first, completing its report in 2021. BER's Advisory Committee (BERAC) was next, followed by the Advanced Scientific Computing Research Advisory Committee.

This report describes BERAC's assessment in response to the charge letter (see p. ii). To develop this document, the BERAC Subcommittee on International Benchmarking has drawn heavily on the BESAC report (BESAC 2021), as it provides an excellent model for addressing the four questions posed in BERAC's charge. In particular, BESAC's insights into the most effective methodology for quantitative and qualitative metrics strongly influenced this report. Here, the BERAC subcommittee seeks to (1) benchmark BER's programmatic investments and science contributions over the last decade and (2) provide actionable recommendations to realize emerging science opportunities over the next decade.

The subcommittee's benchmarking approach combines quantitative metrics (e.g., bibliometric data and programmatic funding) and qualitative metrics (e.g., responses from expert interviews, town hall discussions, and feedback from a public Request For Information). The quantitative metrics provide a means for benchmarking BER's practices, structures, protocols, and resource investment, as well as the products and outcomes of supported science. The qualitative metrics provide diverse perspectives on national and international leadership, horizon scans for emerging opportunities, and broader workforce insights into how BER can attract and retain the top scientific talent necessary for ensuring future international leadership. Data and analyses for these findings and recommendations were gathered and developed in 2021. BER has independently acted in some cases during 2022 to address some of the issues raised.

Overall, BER's international leadership is well-substantiated across its mission areas and enabling

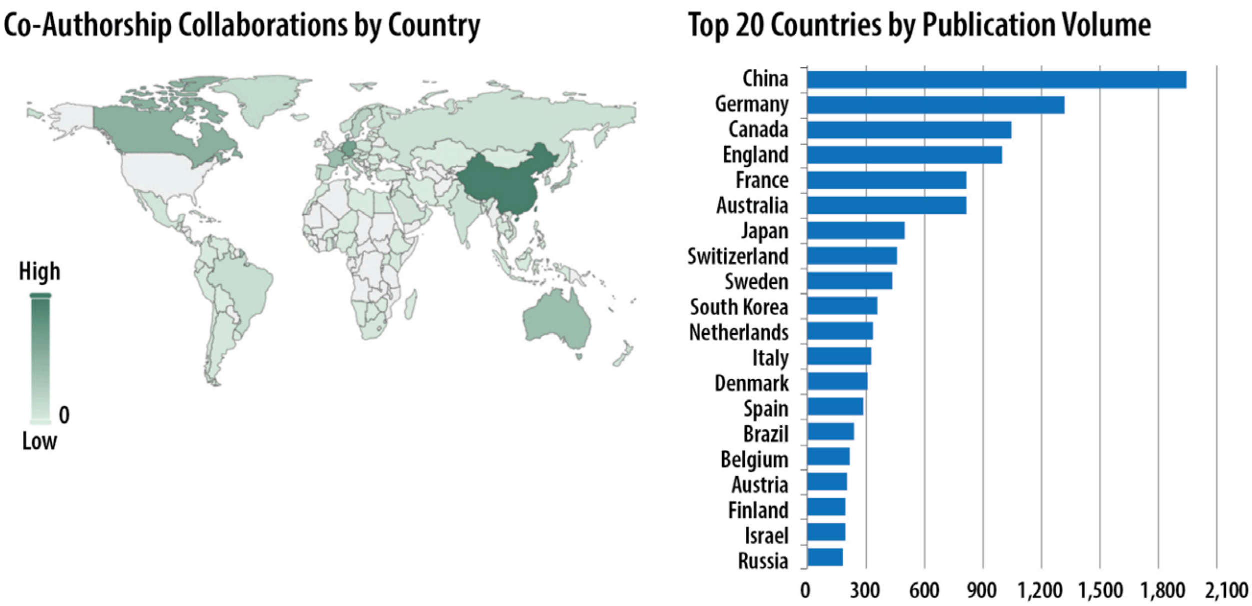


Fig. ES.1. International Collaborations and Publication Volumes by Country Involving BER-funded Scientists. [Courtesy DOE Office of Scientific and Technical Information]

infrastructure. However, this report's key findings and recommendations underscore that BER's continued leadership, as well as that of the broader U.S. research enterprise, should not be taken for granted. The next decade could see the realization of forewarned declines in U.S. scientific competitiveness and leadership noted in previous reports (NASEM 2007; Augustine and Lane 2021) and similarly emphasized in the BESAC report (BESAC 2021). Feedback from experts surveyed across BER mission areas also indicates that volatility in priorities, funding, and workforce retention significantly threatens BER's ability to sustain its leadership. Moreover, BER funding over the past decade has not increased commensurately with the growing scale and acuteness of the national and global challenges that its research addresses. Transformative, high-risk research[1] is required to tackle these challenges and maintain U.S. international competitiveness. The current era is one in which "… our nation cannot afford to miss opportunities, discoveries, and new frontiers that can result from bold, unfettered exploration and freedom of thought that challenges our current understanding of natural processes" (NSB 2007).

Although BER's research leadership is far-reaching and responsible for a range of cutting-edge breakthroughs, the experts did not associate these breakthroughs distinctly with BER. This lack of visibility in the research community is a missed opportunity to recruit a diverse, committed, and exceptional future workforce to BER's research mission.

Finally, many experts noted that international leadership should not be seen as adversarial. Rather, BER's research portfolio should be viewed through a collaborative lens, as it contributes to the collective commons of enabling knowledge for the world. Indeed, many of BER's impactful discoveries are generated through international partnership as shown by the subcommittee's bibliometric metric analyses (see Fig. ES.1, this page). Moreover, BER's goals of combating climate change, transitioning from fossil fuels to renewable

[1] "Transformative research is defined as research driven by ideas that have the potential to radically change our understanding of an important existing scientific or engineering concept or leading to the creation of a new paradigm or field of science or engineering. Such research is also characterized by its challenge to current understanding or its pathway to new frontiers" (National Science Board, National Science Foundation 2020).

resources, and achieving a sustainable bioeconomy that will ensure future prosperity are also societal goals that must be achieved on a global scale.

This report is organized by BER's main mission areas: bioenergy and environmental microbiomes, biosystems design, environmental system science, and climate science. Ch. 2–5 present mission area–specific findings and recommendations. Ch. 6 outlines the contributions of BER-supported user facilities and infrastructure to national and international science leadership. Ch. 7 evaluates and explores opportunities for integrative science across mission areas and potential innovations to amplify BER's scientific impact. Collectively, these chapters answer the first question of the charge letter: What is the international standing of BER's science, and how can BER's leadership be strengthened? Ch. 8 addresses the remaining three charge letter questions focused on issues of workforce recruitment, international partnerships, and research enterprise management and operation (see Appendix A: Key Findings and Recommendations, p. 141).

Overarching Findings and Strategic Recommendations

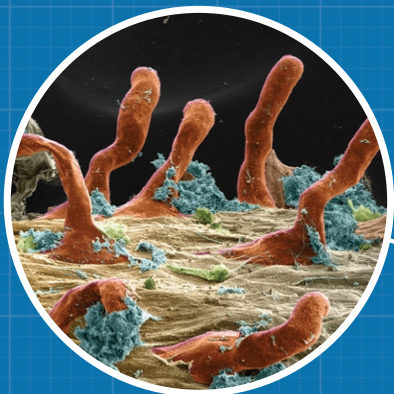
Here, the subcommittee presents overarching findings and recommendations for the next decade, identified by consensus across the full BERAC subcommittee (see Appendix B, p. 150) and experts interviewed for this assessment. With these strategic recommendations, the subcommittee seeks to mitigate a series of risks to BER's continued international leadership in the next decade.

Overarching Findings

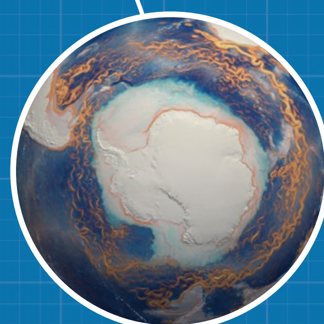
- BER's international leadership is well-substantiated across mission areas and enabling infrastructure.
- Mission areas increasingly target the critical challenges of the coming decades for which Big Science can and must be entrained.
- International leadership is a more meaningful goal when viewed in a collaborative versus adversarial context.
- Future leadership is not guaranteed and will require increased investments and strategic partnerships with private, public, and academic institutions; other DOE programs; other federal agencies; international collaborators; and across disciplines.
- Volatility in priorities, funding, and workforce retention significantly threatens BER's ability to sustain its leadership.
- BER's funding over the last decade has not increased commensurately with the growing scale and acuteness of the national and global challenges that BER missions and science address.
- The science community does not widely associate BER with the major research impacts and achievements it has enabled.

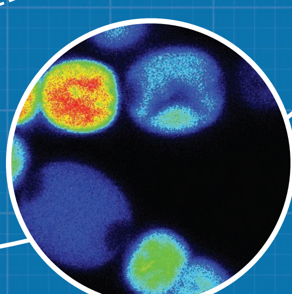
Strategic Recommendations

- Increase and sustain needed resources in all mission areas and in integrative science opportunities across and between these areas (risk: failure to invest).
- Improve connection between basic science and research across Technology Readiness Levels (risk: failure to capitalize on investment).
- Establish horizon-scanning mechanisms for long-range, strategic infrastructure and mission-area investments (risk: failure of imagination).
- Elevate the stature of BER mission science to ensure recruitment of the best and brightest (risk: failure to inspire).
- Prioritize, with time and investment, a culture that supports diversity and inclusion, enables early and mid-career professional development, and delivers the future workforce (risk: failure to sustain future leadership).



CHAPTER 1
Introduction





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Additional Contributors

Margaret S. Torn, *Lawrence Berkeley National Laboratory*
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Efi Foufoula-Georgiou, *University of California–Irvine*

1 Introduction

1.1 BER Research Landscape and Assets

The Biological and Environmental Research (BER) program within the U.S. Department of Energy's (DOE) Office of Science supports transformative basic research and scientific user facilities aimed at achieving a predictive understanding of complex biological, Earth, and environmental systems spanning scales from the molecular to planetary (see Fig. 1.1, p. 3). This fundamental research is advancing understanding of the relationships between energy and environment, contributing to a future of reliable, resilient energy sources and evidence-based climate solutions.

BER is organized into two divisions:

- The Biological Systems Science Division (BSSD) supports fundamental science to understand, predict, manipulate, and design biological systems that underpin innovations for bioenergy and bioproduct production and to enhance the understanding of natural, DOE-relevant environmental processes (U.S. DOE 2021a). Within its systems biology portfolio, BSSD supports genomic science, proteomics, metabolomics, structural biology, computational modeling, and bioimaging research and the application of these approaches to plants, microbes, and communities.
- The Earth and Environmental Systems Sciences Division (EESSD) supports research to characterize and understand feedbacks between Earth and energy systems, including studies on atmospheric physics and chemistry, ecosystem ecology, and biogeochemistry. The division also supports efforts to develop, validate, and analyze Earth system models that integrate information on the biosphere, atmosphere, terrestrial land masses, oceans, sea- and land-ice, subsurface, and human components to advance scientific understanding and improve Earth system predictability.

Both divisions are working to integrate deep-learning and artificial intelligence approaches into their portfolios to accelerate knowledge gained from "Big Data," a hallmark of systems biology and Earth systems science.

To promote world-class research, BER operates three national user facilities that enable observation and measurement of atmospheric, biological, and biogeochemical processes: the DOE Atmospheric Radiation Measurement (ARM) user facility, Environmental Molecular Sciences Laboratory (EMSL), and Joint Genome Institute (JGI).

- ARM provides highly instrumented ground stations at various locations around the globe, mobile measurement resources, and aerial vehicles to continuously measure cloud and aerosol properties and their impacts on Earth's energy balance. ARM measurements have set the standard for long-term climate research observations and provide an unparalleled resource for examining atmospheric processes and evaluating Earth system model performance.
- EMSL, located at Pacific Northwest National Laboratory, provides users with a problem-solving environment by integrating premier instrumentation with high-performance computing and optimized codes. This integration of capabilities enables research teams or individual investigators to unravel the fundamental physical, chemical, and biological mechanisms and processes that underpin larger-scale biological, environmental, and energy challenges.
- JGI, located at Lawrence Berkeley National Laboratory, sequences more than 450 trillion DNA bases per year. This user facility provides state-of-the-science capabilities for genome sequencing, synthesis, metabolomics, and analysis. With nearly 1,600 users worldwide on active projects, JGI is the preeminent resource for sequencing plants, fungi, algae, microbes, and microbial communities foundational to energy and environmental research.

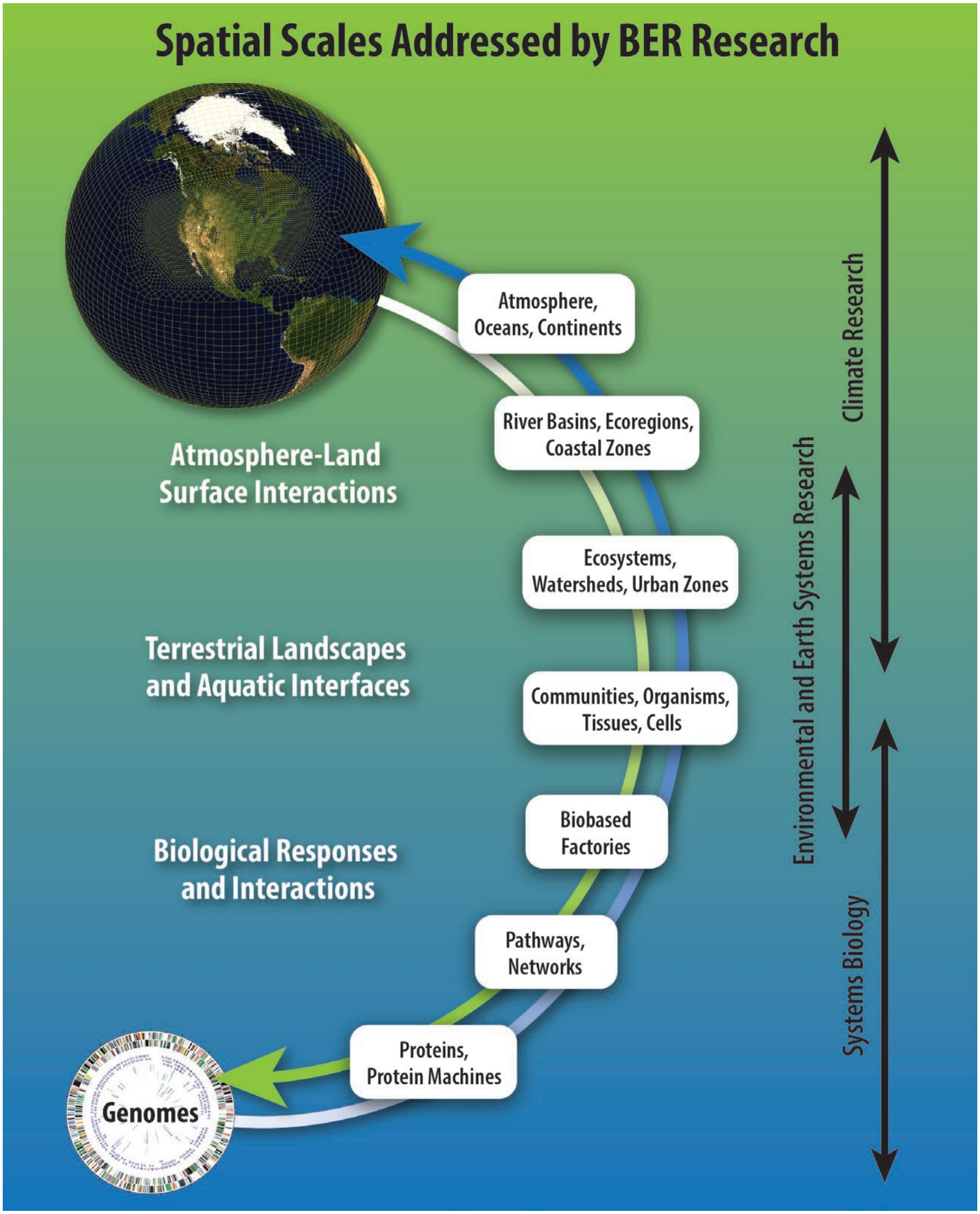


Fig. 1.1. Spatial Scales Addressed by BER Research. BER research spans a broad range of natural systems. These systems are not only structurally and spatially complex, with many different interacting parts spanning molecular to global scales, they also are dynamically complex, encompassing processes that occur over time scales ranging from nanoseconds to centuries.

BER also supports a suite of experimental technologies, methodologies, instruments, and computational capabilities at DOE light, neutron, and cryo-EM facilities that are available to users. In addition to these resources, BSSD supports a Bioimaging Science Program, which aims to develop new imaging and measurement technologies to visualize the spatial and temporal relationships of key metabolic processes governing phenotypic expression in plants and microbes. The activity includes efforts to incorporate concepts enabled by quantum information science into new approaches for imaging and characterization and to advance design of sensors and detectors based on correlated materials for real-time biological and environmental sensing technologies.

Additionally, EESSD supports an extensive data management activity, encompassing both observed and model-generated data collected by environmental field experiments on behalf of DOE and the international community. This activity also archives information generated worldwide by climate and Earth system models of various complexity and sophistication.

1.2 BER Research Operations and Management

BER manages an annual research portfolio of about $750 million that encompasses research, facilities, and infrastructure (see Fig. 1.2, p. 5). The program uses several funding modalities to support work at universities, national laboratories, and research institutions across the country. Grantees include individual principal investigators, small teams of investigators, and four Bioenergy Research Centers (BRCs), which collectively support hundreds of researchers. The BRCs are funded at $25 million to $30 million per year as multi-institutional, interdisciplinary team-science efforts to develop novel feedstocks and microbial conversion processes for a sustainable biomass-to-biofuels pipeline.

1.2.1 University and National Laboratory Projects

Awards to researchers at universities and other non-federally funded research and development centers are typically for up to 3 years and total less than $1 million. At the national laboratories, BER funds Science Focus Areas (SFAs), which are multidisciplinary, multi-investigator, long-term projects renewed every 3 to 4 years. Funded at $1 million to $8 million annually, the national laboratory–led SFAs may often include collaborators from universities, DOE user facilities, and other national laboratories. The purpose of the decadal SFA structure is to encourage, facilitate, and effectively manage integrative and collaborative programs that conduct high-quality scientific research and achieve solutions in support of BER goals. SFAs are structured to take advantage of national laboratory strengths to conduct coordinated, team-oriented research in a manner distinct from, but complementary to, research conducted at other institutions. BER supports additional long-term national laboratory projects, such as the Next-Generation Ecosystem Experiments (NGEEs), allocating funding to a lead national laboratory that then distributes it to selected partners that may include other national laboratories, universities, and institutions. Both these national laboratory funding modalities are unique to BER.

1.2.2 Community Infrastructure Projects

BER's community research infrastructure projects include the (1) DOE Systems Biology Knowledgebase (KBase), a software and data science platform for systems biologists; (2) National Microbiome Data Collaborative (NMDC), an open-access framework that facilitates more efficient use of microbiome data for applications in energy, environment, health, and agriculture; (3) Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) for data management; (4) AmeriFlux Management Project for the AmeriFlux network; (5) Earth System Grid Federation (ESGF), an interagency distributed data and computational platform led by DOE that supports the international Earth system science community; and (6) multilaboratory collaborations for community cyberinfrastructure, exemplified by the Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds project (see Case Study, p. 57).

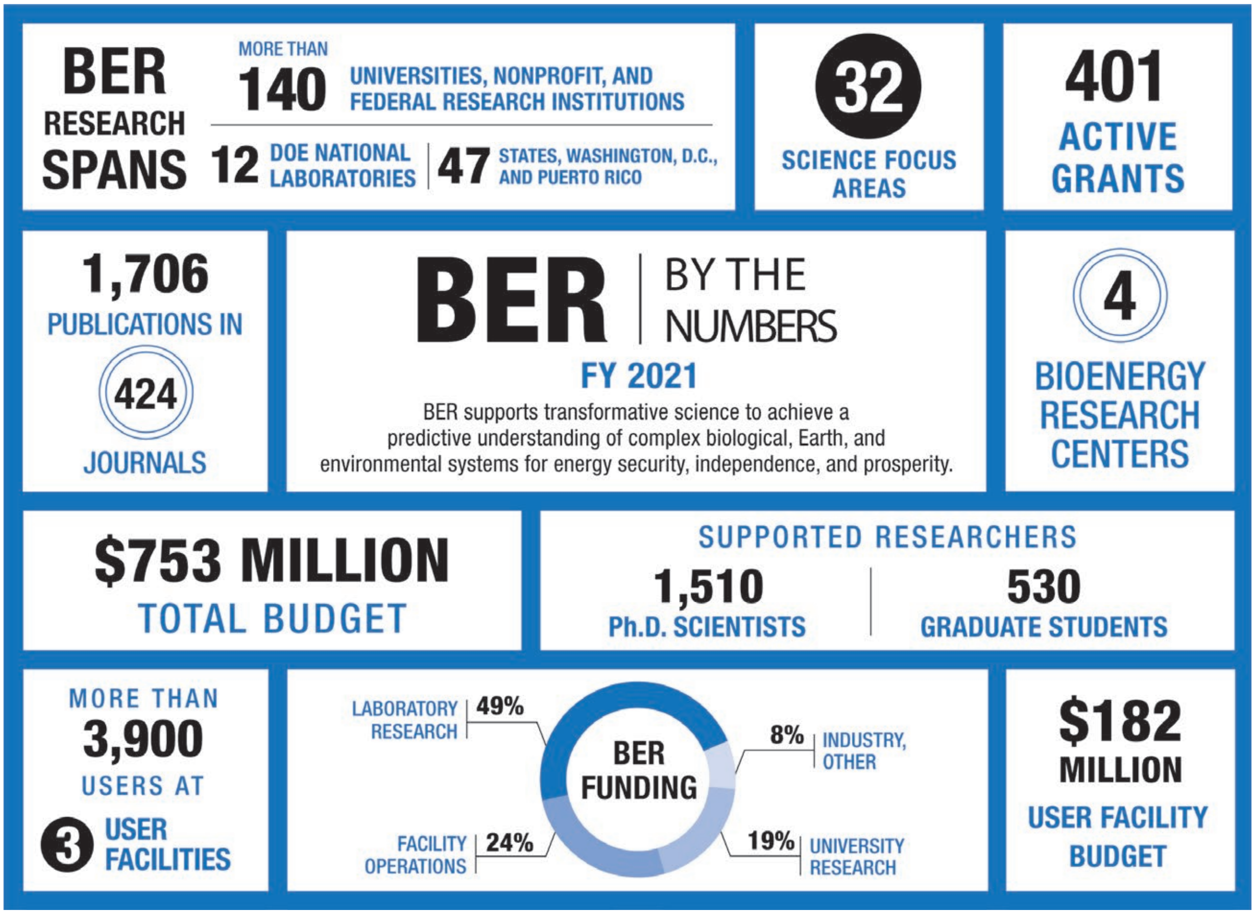


Fig. 1.2. BER by the Numbers. BER manages an annual research portfolio of about $750 million that encompasses research, facilities, and infrastructure.

1.2.3 Small Business Innovation and Tech Transfer

BER also provides grants through the federal Small Business Innovation Research and Small Business Technology Transfer (SBIR/STTR) programs to help certain small businesses conduct research and development (R&D). Projects must have the potential for commercialization and meet DOE mission–specific R&D needs. Recent BER SBIR/STTR calls for proposals focused on urban measurement technology, advanced data analytical technologies for systems biology and bioenergy, structural biology tools for characterizing microbial and plant systems relevant to bioenergy, imaging technologies for biological systems, and biological approaches and technologies for synthetic polymer upcycling.

1.2.4 Workforce Development

Finally, BER supports scientific leadership development through several Office of Science initiatives. The highly competitive and prestigious Early Career Research Program awards 5-year grants to successful applicants from universities and national laboratories who received their doctoral degrees within the past 10 years. Additionally, the Office of Science Graduate Student Research Program provides 3 to 12 months' support for graduate students to pursue part of their thesis research at a DOE national laboratory or user facility. New programs, such as Reaching a New Energy science Workforce (RENEW), explicitly address issues of workforce diversity, equity, and inclusion by supporting entry of faculty and students at minority-serving institutions into Office of Science mission spaces.

1.3 Defining BER's Leadership, Success, and Reputation

How can we measure BER science and scientific infrastructure on the world stage? Although daunting, this challenge is not impossible, as suggested by studies from the American Academy of Arts and Sciences and the National Academies of Sciences, Engineering, and Medicine (NASEM). The studies indicate that international benchmarking for a research field (NASEM 2000) and for the national research enterprise (AmAcad 2020) is both feasible and valuable, providing a sketch of research status and future directions.

To conduct such an assessment in response to the Office of Science charge, the BER Advisory Committee's (BERAC) Subcommittee on International Benchmarking established working groups in BER mission areas. Each group comprised six to eight members and co-leads, including international participants, with deep expertise spanning various institutions and backgrounds. The working groups identified international peer groups and BER-relevant focus areas for comparison. The collective goal was to benchmark performance in the last decade and to help inform BER's strategy in the next decade with actionable recommendations (see Appendix A: Key Findings and Recommendations, p. 141).

The subcommittee also identified a series of case studies that capture takeaway messages from the team's assessment (see Table 1.1, p. 7). These focused stories are intended to illustrate the high-impact successes, challenges, and future opportunities for BER and its research community.

In examining BER leadership, the subcommittee structured its assessment around several questions:

- Is BER-supported research fundamentally advancing science? If so, is this impact largely internal or at an international level?
- Are BER-pioneered scientific approaches at the cutting edge and influencing scientific research more broadly?
- Are BER-supported scientists regarded as thought leaders in the global research community?
- Is BER making the necessary investments—in research, infrastructure, and training the next generation of scientists—that position it to lead now and in the future?

1.4 Assessment Methodologies Used for Benchmarking

The Basic Energy Sciences Advisory Committee's (BESAC) international benchmarking report (BESAC 2021) described a benchmarking methodology incorporating analyses of bibliometric data, interviews with experts, and community engagement at conferences. Using this methodology as a roadmap, the BERAC subcommittee analyzed both quantitative bibliometrics to provide a snapshot of research performance over the past 10 years and qualitative assessments of leadership to provide a foundation for horizon scanning in BER mission areas.

1.4.1 Publication and Funding Analyses

In addition to bibliometric data from public databases, such as citations and international authorships of publications, the BERAC subcommittee examined funding levels over time as another measure of BER commitment and investment in scientific leadership. The subcommittee is deeply grateful to staff at DOE's Office of Scientific and Technical Information for conducting bibliometric searches and compiling data for BER-supported scientists compared to other U.S. and non-U.S. authors across BER mission domains (see Appendix C: Approach to Metrics and Methodologies, p. 151).

Not all potentially relevant metrics were available for this evaluation. For example, some data and software citations were too new to be applied or tallied comprehensively. Also, because BER research spans many topics, activities, and communities and given the time constraints for conducting this study, the working groups did not evaluate some potential indicators of leadership, such as (1) authorship of key reports (e.g.,

Table 1.1 Case Studies and Takeaways			
Title	**Mission area**	**Takeaways**	**Page**
DOE Bioenergy Research Centers	Bioenergy and Environmental Microbiomes	Well-managed, mission-inspired scientific centers can be successful, and sustained collaborative funding can increase research impacts.	p. 16
From Biofuels to Bioeconomy—DOE Funding Helps Gingko Develop Leading Cell Programming Platform	Biosystems Design	DOE-funded workforce training outside of PhD tracks (e.g., associate degrees, apprenticeships, and certificates) is essential for the future bioeconomy.	p. 36
Amyris—Delivering on the Promise of Synthetic Biology	Biosystems Design	Partnerships with R&D companies can amplify BER research impacts and bring BER-relevant processes to scale for market impact.	p. 39
Next-Generation Ecosystem Experiments	Environmental System Science	Explicitly connecting understanding of ecosystem processes to Earth system modeling is a paradigm shift in the integration of modeling, experimentation, and observations.	p. 51
IDEAS—Interoperable Design of Extreme-scale Application Software	Environmental System Science	A community approach has enabled leadership in the computational modeling of terrestrial and watershed ecosystems with high process fidelity at various spatial scales.	p. 57
CMIP—Coupled Model Intercomparison Project	Climate Science	BER support of and leadership in CMIP has been vital to the project's far-reaching success in the international climate science community.	p. 73
Cloud Feedbacks and Climate Sensitivity	Climate Science	BER is a world leader in understanding how clouds affect Earth's energy budget, how and why their properties shift under climate change, and how sensitive Earth is to carbon dioxide.	p. 76
The National Virtual Biotechnology Laboratory—DOE's R&D Response to COVID-19	Enabling Infrastructure	An enabling infrastructure coupled with diverse capabilities can be leveraged for a rapid, impactful response to national needs or emergencies.	p. 95
Can BER Influence National Laboratory Culture to Attract Great Talent?	People, Partnerships, and Productivity	DOE and the national laboratories need to prioritize, with time and investment, workforce development.	p. 127
MOSAiC—Multidisciplinary Drifting Observatory for the Study of Arctic Climate	People, Partnerships, and Productivity	The Atmospheric Radiation Measurement user facility demonstrated BER's key leadership in an international partnership by operating a major component of the largest Arctic scientific expedition in history involving more than 80 research institutions from 20 countries.	p. 133

by NASEM and Intergovernmental Panel on Climate Change), (2) leadership in significant workshops, or (3) keynote talks at major conferences. Future benchmarking efforts could consider these indicators.

1.4.2 Community Input

Since quantitative metrics are insufficient for assessing leadership and scientific advancement, the subcommittee sought input from thought leaders and scientists representing all BER research domains and from different institutions, countries, and career stages. The subcommittee used these interviews with national and international experts as a primary means to assess BER's potential for international leadership in the next decade. As scientists, subcommittee members are deeply concerned about overextrapolating the findings from small sample sizes, but they captured many interesting comments from more than 60 interviews. The team then analyzed these comments to form hypotheses, and, when similar messages were heard from multiple experts, they gained confidence in a hypothesis and sought quantitative data or conducted additional interviews when possible. The subcommittee also reported instances where there was a lack of consensus or where a comment seemed particularly insightful.

To test the collected hypotheses, the team also elicited feedback from a larger pool of BER stakeholders through town halls with focus groups (e.g., Early Career Program awardees), where participants echoed and amplified many of the experts' comments. The focus groups also provided unique insights on workforce development, recruitment, and talent retention. The subcommittee received additional input in response to a public Federal Register Request For Information (see Appendix D, p. 156).

1.5 Current Status of International Leadership in BER's Mission Space

Predictions from the National Academies "Rising Above the Gathering Storm" report (NASEM 2007) might now be evident in publication and citation trends for BER mission areas (see Ch. 2–7, beginning on p. 11). Although BER holds distinguished leadership across its mission space in terms of generating top-ranked publications and higher citation rates relative to U.S. and international peers, the leadership gap has been closing rapidly since 2010. The research community and stakeholders have raised concerns about the international competitiveness of the U.S. research enterprise over the last 2 decades, and the next decade marks a potential inflection point for U.S. global leadership. This sentiment is mirrored in the National Science Board Vision 2030 report, which notes a "case for urgency" because global R&D "… is growing faster, and consequently the U.S. share of discovery is dropping" (NSB 2020).

One clear symptom of this trend is seen in national research investment over the past decade. As global R&D funding increases to record levels (~$2 trillion as of 2019), the spending gap between the United States, European Union, and China is narrowing rapidly. The United States risks falling out of the top 10 ranked countries in terms of research workforce development rates and R&D expenditures as a percentage of gross domestic product (see Fig. 1.3 and Fig. 1.4, p. 9). Appropriated budgets for BER have remained flat in the last decade when normalized to 2010 dollars despite increased costs of performing research and a larger scientific workforce.

Compounding the impact of flat budgets, major cuts in DOE's 2018 budget request represented the potential for devastating long-term losses to BER science and the BER-supported research workforce (see Fig. 1.5, p. 10). Although final budget appropriations avoided the proposed cuts to critical programs, experts interviewed for this assessment consistently noted the more subtle and long-term effects of these potential cuts on morale, retention, and BER's reputation in recruiting scientists across all levels of seniority. These impacts are particularly concerning in the post-pandemic environment in which many employees are leaving the workforce for reasons that are relational and cultural (e.g., not feeling valued or recognized and not having opportunities for professional and personal growth) rather than transactional (e.g., salary increases and work conditions; De Smet et al. 2021). There is no reason to believe that the scientific workforce is immune

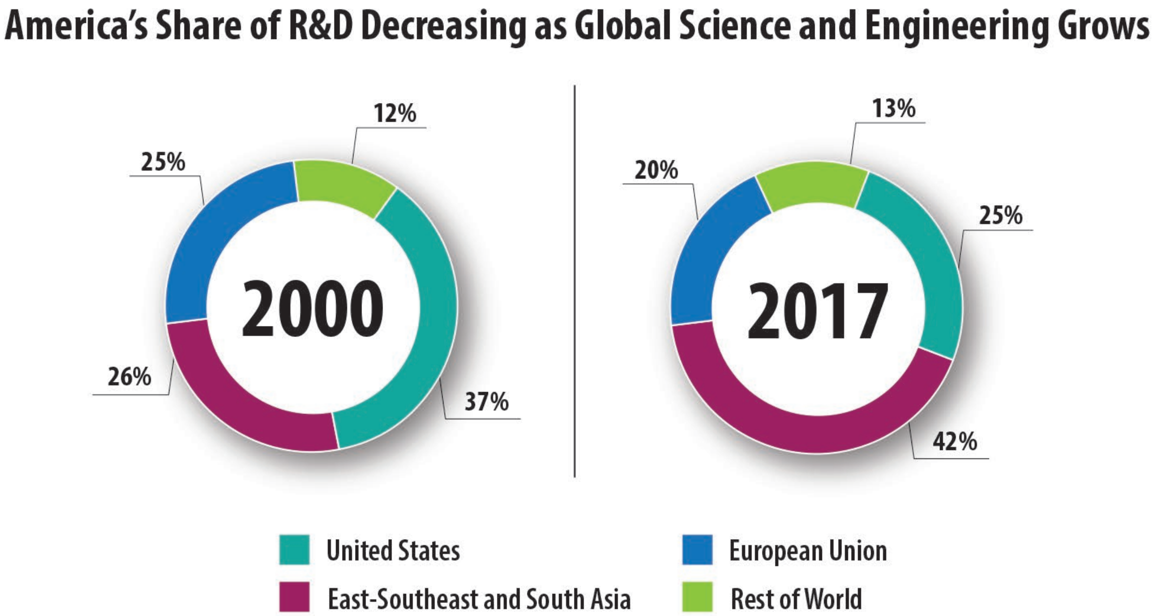


Fig. 1.3. Comparing U.S. and Global Science Investments. While the U.S. investment in research and development (R&D) continues to grow in absolute terms, the investment by other countries is growing faster. As a result, the U.S. share of global R&D spending decreased from 37% to 25% between 2000 and 2017. [Courtesy National Science Foundation]

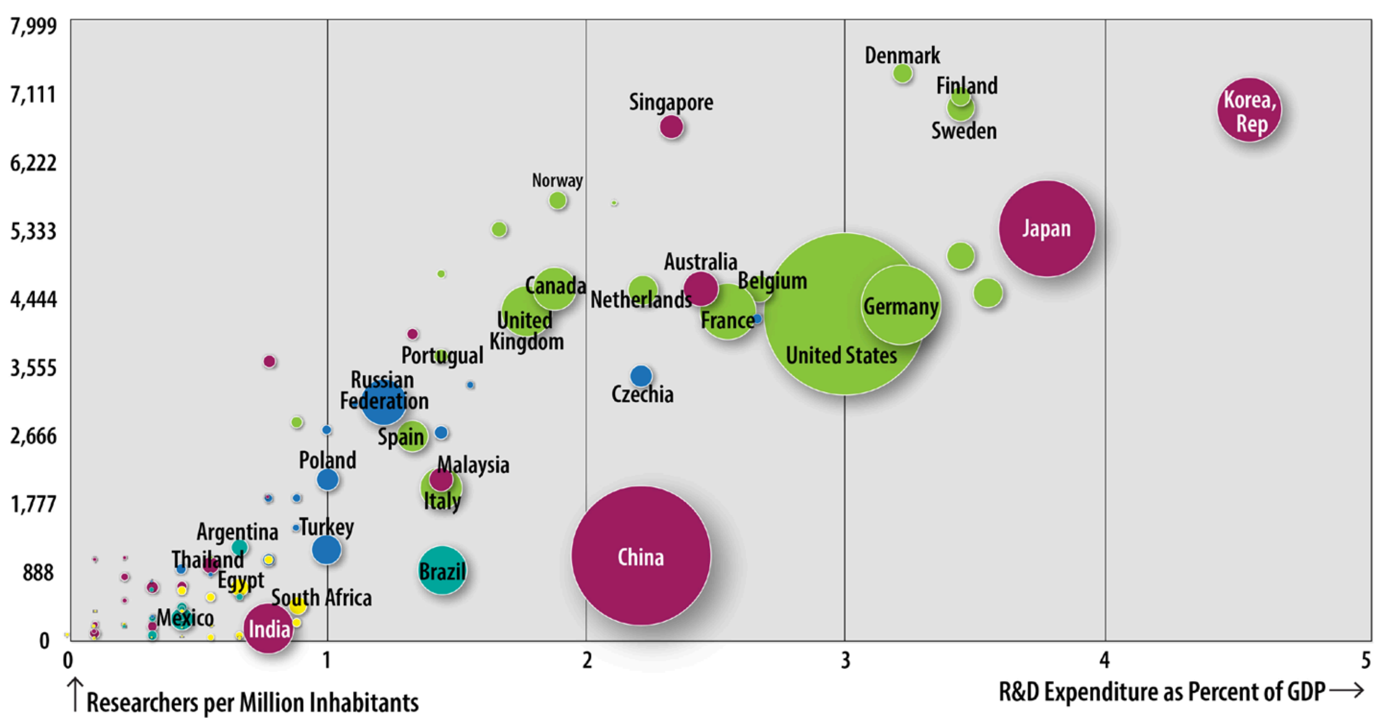


Fig. 1.4. Investments in Global R&D on the Rise. According to the UNESCO Institute for Statistics, global R&D has increased to record levels (~$2 trillion as of 2019) over the past decade. Countries have pledged additional substantial increases in public and private funds as well as the number of researchers by 2030 as part of their response to the United Nation's Sustainable Development Goals. [Courtesy UNESCO. uis.unesco.org/apps/visualisations/research-and-development-spending]

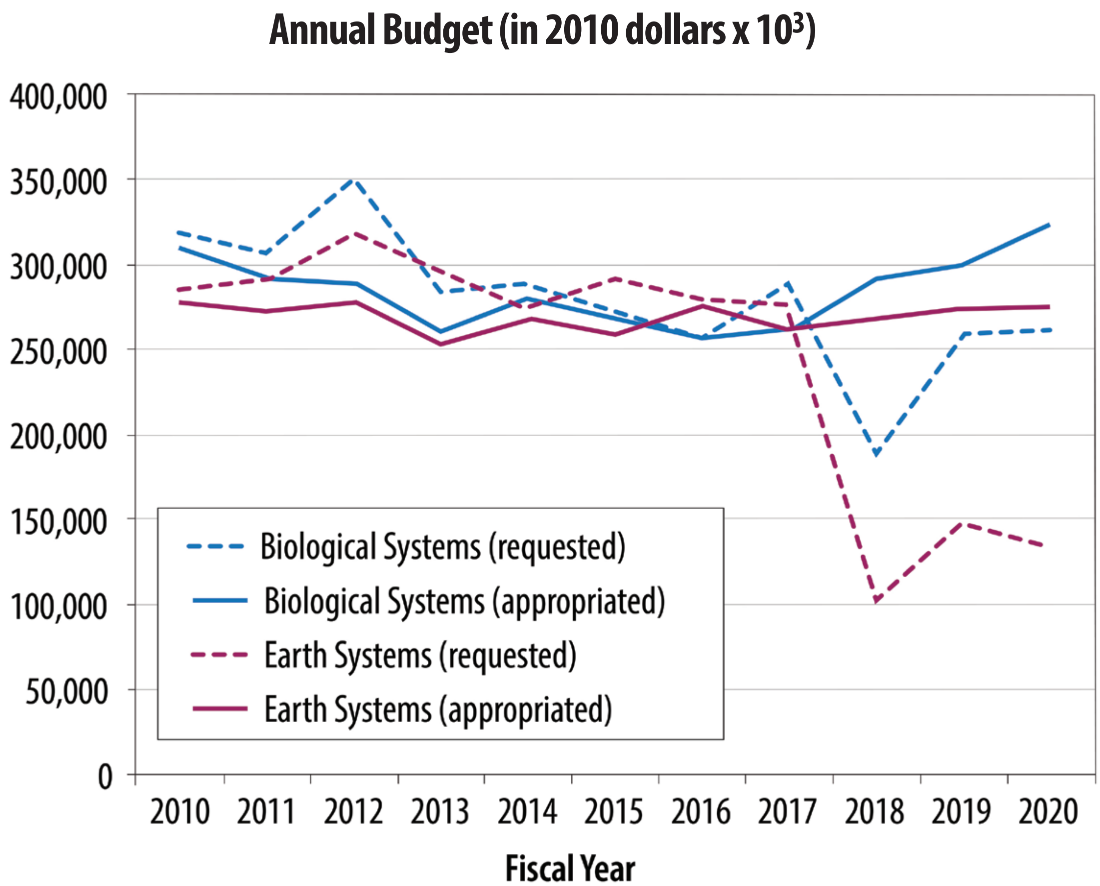
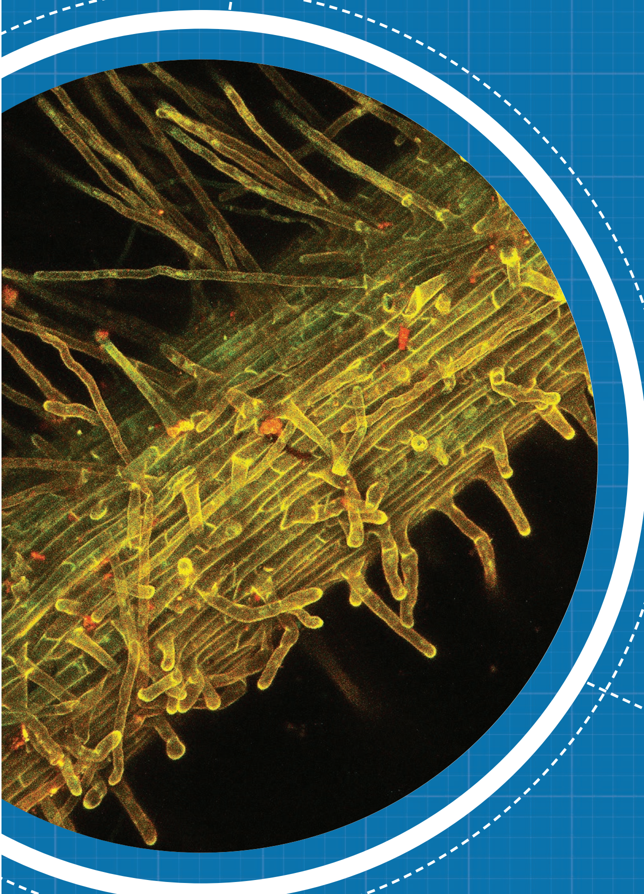


Fig. 1.5. Budget Requests vs. Appropriations by Fiscal Year for BER's Biological Systems Science Division and Earth and Environmental Systems Sciences Division. Although final budget appropriations avoided the major cuts shown in DOE's 2018 budget request, potential cuts still impacted morale, retention, and BER's reputation in recruiting scientists across all levels of seniority, according to interviewed experts. [Courtesy DOE Office of Scientific and Technical Information]

or exempt from this trend (see Case Study: Can BER Influence National Laboratory Culture to Attract Great Talent?, p. 127). Although the stability of flat fiscal appropriations or even slight increases is often a focal point for BER programmatically, BER needs to consider the workforce cultural impacts of potential and realized volatility as a major structural vulnerability.

BER is tackling critical scientific challenges and global risks that no country or funding body has the singular ability to address. This perspective is reinforced by the National Science Board's Vision 2030 report, which emphasized that science and technological breakthroughs are "… now a truly worldwide enterprise, with more players and opportunities from which humanity's collective knowledge is growing rapidly. This dynamic R&D landscape is characterized by interdependence as well as competition" (NSB 2020). To conclude, the BERAC subcommittee emphasizes the critical importance of avoiding a myopic, narrow, and adversarial framing of international leadership for discovery science, the fruits of which must be realized at a global scale.



CHAPTER 2

Bioenergy and Environmental Microbiomes

Working Group Co-Leads

Crysten Blaby, *Lawrence Berkeley National Laboratory*
Brian H. Davison, *Oak Ridge National Laboratory*

Working Group Members

Ana Alonso, *University of North Texas*
Ludmilla Aristilde, *Northwestern University*
Ramon Gonzalez, *University of South Florida*
Janet Jansson, *Pacific Northwest National Laboratory*

Additional Contributors

Maureen McCann, *National Renewable Energy Laboratory*
Massie S. Ballon, *Lawrence Berkeley National Laboratory*

Chapter 2
Key Findings and Recommendations

Key Findings

KF2.1 BER is an international leader in fundamental bioenergy, sustainability, and environmental microbiome research, but other countries are catching up to the United States in scientific leadership and their capacity to translate basic research into practical applications.

KF2.2 BER funding of plant science studies has positioned the United States as the world leader in plant bioenergy and feedstock research.

KF2.3 BER leads in developing and applying genome- and omics-based approaches to bioenergy and environmental microbiome research. Maintaining this position requires continued support for new technologies and experimental testing of hypotheses generated from omics data. The next frontier will be combining multiomics approaches with innovations in microbial and plant biochemistry, areas where BER may lag other countries.

KF2.4 Several nations, including China, may outperform the United States in deploying industrial biotechnological applications, partly due to external policies and market trends, lower investment in fundamental bioprocessing research, and gaps in continuity between discovery, development, and deployment of discoveries. .

KF2.5 The DOE Bioenergy Research Center (BRC) program exemplifies the power of well-managed team science, which benefits from stable funding, a strong mission, and a collaboration emphasis. With well-integrated, multidisciplinary teams, the BRCs excel at performing and publishing research in foundational science and building collaborator networks, but their intellectual property has not been widely deployed.

KF2.6 Interagency calls, when initiated, provide a productive mechanism for fostering research collaborations.

Recommendations

R2.1 Spearhead a renaissance in bioenergy research, the need for which is highlighted by recent geopolitical events including the war in Ukraine and U.S. economic vulnerability to disruptions in the global energy market. To maintain its international position as a research leader, BER should support and encourage the next generation of researchers to embrace innovative, high-risk approaches for achieving bioenergy goals.

R2.2 Lead efforts to provide the fundamental knowledge needed to bring products to market. BERAC does not recommend that BER support applied research, since BER's strength and preeminence lie in fundamental science. However, BER should engage in creative opportunities to catalyze communication between basic and applied researchers to speed transitions between early Technology Readiness Levels.

R2.3 Encourage interactions and interdisciplinary collaborations that better integrate the unique architecture of BER's research portfolio and provide the research community with access to established resources such as ongoing perennial field experiments and their growing data collections. These activities will generate knowledge between and across disciplines and experimental scales, from computation to experimentation and from molecules to phenotypes.

R2.4 Build on genome-enabled bioenergy and environmental microbiome leadership and knowledge to understand the complex interactions between bioenergy crops and environmental microbiomes, thereby informing sustainable management of ecosystems under climate change.

2 Bioenergy and Environmental Microbiomes

2.1 Overview of BER's Genomic Science Program

The Genomic Science Program (GSP), within BER's Biological Systems Science Division (BSSD), supports a multidisciplinary research portfolio grounded in the genomic sciences. GSP pursues fundamental research to understand, predict, manipulate, and design plant and microbial systems for innovations in renewable energy, insights into environmental processes, and biotechnological breakthroughs supporting the U.S. bioeconomy. Research supported by GSP is multiscaled and complex, encompassing the functions of atoms in protein structures, the systems biology of bioenergy crops and their microbiomes, feedstock conversion technologies, and environmental microbes and their communities. GSP research contributes to a genome-based foundation critical for sustainable bioenergy development in a changing climate.

The program's multimodal approach to science funding leverages the strengths of DOE scientific user facilities, individual researchers, research teams, national laboratories, universities, and research centers. Most GSP project teams include collaborators from these different organizations, creating a framework for highly interdisciplinary research. Universities and other academic institutions typically receive funding through shorter-term awards (usually 3 to 5 years) and collaborations with national laboratory–led projects. At the national laboratories, GSP funds researchers as user facility staff and through the Bioenergy Research Centers (BRCs) and Science Focus Areas (SFAs). Across seven national laboratories, GSP currently supports 14 SFAs, which are team-oriented research projects that take advantage of the laboratories' distinctive strengths for conducting collaborative, coordinated, and sustained research programs.

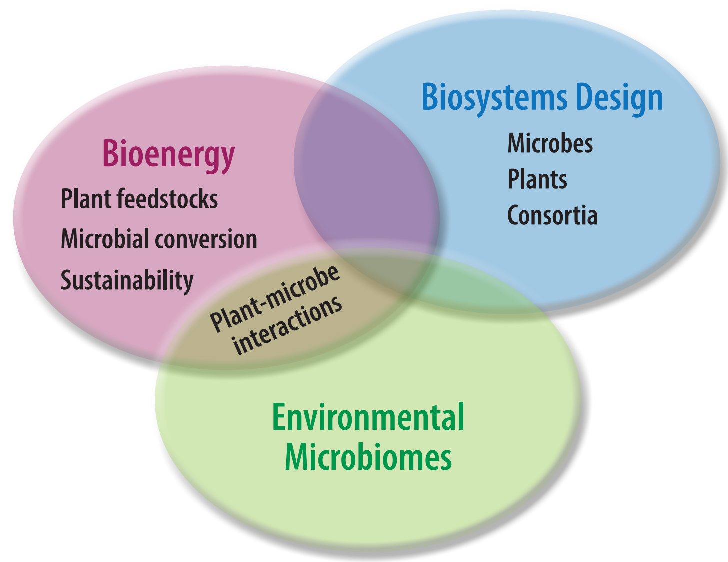


Fig. 2.1. Genomic Science Program's Primary Research Areas. These areas intersect significantly in terms of the microbes, plants, and communities under investigation and the basic tools used for genomics, molecular characterization and imaging, and computational biology. Environmental Microbiome research also intersects with programs in BER's Earth and Environmental Systems Sciences Division.

2.1.1 GSP Primary Research Areas

GSP research is broadly grouped into three areas: Bioenergy, Environmental Microbiomes, and Biosystems Design. Each is integrated with other portfolio elements, such as enabling capabilities and user facilities, through targeted, crosscutting funding opportunities and DOE national laboratory projects. Considerable synergy exists among the three areas in addition to independent topical foci (see Fig. 2.1, this page).

This chapter reports on the BERAC subcommittee's assessment of the international competitiveness of the Bioenergy and Environmental Microbiome research areas, while Ch. 3, p. 29, focuses on Biosystems Design.

Bioenergy

Bioenergy research provides the foundational genomics-based knowledge needed to produce and deconstruct renewable plant biomass and convert it to sustainable fuels, chemicals, and other bioproducts. The GSP Bioenergy portfolio supports the development of innovative approaches for sustainable bioenergy production by accelerating systems biology–based understanding of (1) nonfood plants that can serve as dedicated bioenergy feedstocks and (2) microbes that can break down plant cellulosic biomass and synthesize biofuels and bioproducts.

The Bioenergy portfolio encompasses three research subareas—plant genomics, microbial conversion, and sustainable bioenergy—and four BRCs led by either a DOE national laboratory or top university. The mission of the BRC program is to break down the barriers to actualizing a domestic bioenergy industry. The centers take distinctive approaches toward the common goal of accelerating the pathway to improving and scaling up advanced biofuel and bioproduct production processes.

Environmental Microbiomes

Environmental Microbiome research seeks to understand how microbes and plants interact in their natural environments. Of particular interest is the ability to predict these interactions based on organisms' genomic information and the dynamic expression of their activities within a community. Gaining a predictive and functional understanding of microbiomes will enable insights into microbial ecology, plant-microbe interactions, and element cycling in terrestrial environments. The research community continues to learn how environmental microbiomes, such as in soil and plant roots, play a direct role in mitigating species and ecosystem responses to stress from drought and other potential climate change impacts.

Biosystems Design

Biosystems Design efforts focus on accelerating the ability to securely design, build, and control plants and microbes for beneficial uses such as clean energy, biomaterials production, and carbon sequestration. Underpinning these goals is research to advance fundamental understanding of genome biology and to develop the genome-scale engineering technologies needed for these purposes.

2.1.2 GSP Enabling Capabilities

GSP enabling capabilities consist of (1) computational biology and cyberinfrastructure, (2) biomolecular characterization and imaging science, and (3) scientific user facilities. These capabilities add considerable strength to GSP's funding model and international competitiveness, empowering the program to support more than 10,000 researchers directly or indirectly per year. This achievement is remarkable considering the relatively small budget of BSSD compared to other DOE programs that support user facilities.

- **Computational Biology and Cyberinfrastructure.** Open-access and integrated computational capabilities tailored to large-scale data science investigations for molecular, structural, genomic, and omics-enabled research on plants and microbes for a range of DOE mission goals. GSP cyberinfrastructure resources include the DOE Systems Biology Knowledgebase (KBase), National Microbiome Data Collaborative (NMDC), and Joint Genome Institute (JGI).
- **Biomolecular Characterization and Imaging Science.** Imaging and measurement technologies enabling visualization of the relationships among biomolecules, cellular compartments, and higher-order biological systems.
- **DOE Scientific User Facilities.** Integrated capabilities across user facilities and resources for genome sequencing and analysis, DNA design and synthesis, molecular sciences, structural biology, and imaging. BER-supported user facilities and resources include: JGI, the Environmental Molecular Sciences Laboratory (EMSL), and structural biology and imaging resources at DOE synchrotron and neutron facilities.

Another unique and commendable product of GSP-sponsored research and user facilities is the generation of large-scale genome and genome-based resources, which contribute unprecedented value to research fields and communities. These resources have transformed research from laborious experiments examining only one protein or organism at a time to computational analyses that simultaneously compare diversity across the tree of life and to multiscale population-wide experiments that generate predictive insights. For several decades, these GSP-funded, large-scale, genome-based resources have enabled a shift in bioenergy and environmental microbiome research from description to prediction and redesign.

2.1.3 Assessment Approach

This chapter provides a general assessment of BER international leadership and competitiveness in bioenergy and environmental microbiome sciences. For bioenergy, specific attention is given to plant sciences and systems biology, two core topics in GSP's Bioenergy research portfolio. Environmental Microbiomes research is included in this assessment because such studies can potentially bridge ecosystem processes with microbial-mediated biogeochemical cycling in soils, yielding insights for optimizing bioenergy crop productivity and environmental sustainability. A case study of the BRCs presents an example of unique multidisciplinary teams whose research spans these topics and more (see Case Study: DOE Bioenergy Research Centers, p. 16).

For this assessment, BERAC consulted thought leaders from the United States and abroad whose collective expertise spans bioenergy, microbiomes, plants, facility management, metabolic engineering, fundamental and applied sciences, and capital investment in energy solutions. These interviews helped generate hypotheses about BER's international competitiveness that were evaluated in a virtual town hall by early to mid-career scientists who had received BER Early Career Research Program awards. Breakout groups discussed the hypotheses generated by thought leaders as well as other aspects of BER's international competitiveness evident to early career researchers.

2.2 Bioenergy Leadership Status

2.2.1 Successes and Impact

BER leads the world in systems biology, genomics, and genome-based approaches to understanding energy-relevant organisms and processes. It is recognized as an international leader in developing and applying omics technologies; acquiring and integrating large-scale resources, such as whole-genome and metagenome sequences, transcriptomes, and population-wide genetic inventories; and providing researchers with unique capabilities at DOE user facilities. BER also exhibits strength in metabolic engineering and synthetic biology research and supports several pioneers in these fields, especially for valuable nonmodel organisms. Uniquely, BER places bioenergy in an environmental context with a research portfolio that encompasses field- and laboratory-based studies, individual- and population-centric studies, computation and experimentation, and research scales ranging from genes to genomes to biogeochemical cycling involving microbial communities and ecosystem-level structures.

The impact of BER-sponsored research penetrates domains beyond bioenergy. BER's publications and research products, such as genome sequences and analytical tools, have shifted paradigms in the study of biology (see Box 2.1, Poplar Genome Sequence Sprouts Discoveries, p. 19). Some notable examples from the last decade include:

- Development of bioenergy feedstocks with both high yield and improved composition and convertibility (Sun et al. 2021; Bastiaanse et al. 2019; Biswal et al. 2018; Yoo et al. 2018; Dumitrache et al. 2017).
- Emergence of lignin as a value-added product based on improved understanding of its role and behavior in plant cell-wall synthesis, feedstock pretreatment, and microbial conversion of feedstocks (Ragauskas et al. 2014; Zhuo et al. 2022; Yu et al. 2021; Dixon and Barros 2019; Notonier et al. 2021; Salvachua et al. 2020).
- Development of perennial and cover crop feedstock genomics for gene validation and accelerated breeding, as well as linkages between feedstocks and their microbiomes (Lovell et al. 2021; Banda

Continued on p. 18

CASE STUDY

DOE Bioenergy Research Centers

genomicscience.energy.gov/bioenergy-research-centers

BER's four Bioenergy Research Centers (BRCs) demonstrate that well-managed mission-inspired science centers can drive major advances in the production and conversion of lignocellulosic feedstocks to biofuels and bioproducts and that sustained collaborative funding increases overall science impact.

The mission of the BRCs was largely defined in a 2006 roadmap titled "Breaking the Biological Barriers to Cellulosic Ethanol" (U.S. DOE 2006). Late the following year, the first three centers began operating: Great Lakes Bioenergy Research Center (GLBRC), Joint BioEnergy Institute (JBEI), and BioEnergy Science Center (BESC). The program was renewed in 2017 with the Center for Bioenergy Innovation (CBI) succeeding BESC and the addition of the Center for

Continued on next page

Takeaway

Well-managed, mission-inspired scientific centers can be successful, and sustained collaborative funding can increase research impacts.

DOE Bioenergy Research Center Strategies at a Glance

Overcoming the critical basic science challenges to cost-effective production of biofuels and bioproducts from plant biomass requires the coordinated pursuit of numerous research approaches to ensure timely success. Collectively, the DOE Bioenergy Research Centers provide a portfolio of diverse and complementary scientific strategies that address these challenges. These BRC strategies are listed briefly below.

	Sustainability	Feedstock Development	Deconstruction and Separation	Conversion
CABBI	Integrate spatially explicit economic and environmental analyses for a sustainable bioeconomy	Develop "plants as factories" for sustainable and resilient production of biofuels and bioproducts	Develop industrially relevant process and extraction technologies for feedstock oils and sugars	Establish artificial intelligence/machine learning–driven biofoundry for biofuels and bioproducts
CBI	Optimize water and nutrient use for high-yielding bioenergy crops with improved soil carbon storage	Create process advantaged bioenergy crops exploiting natural genetic variation found in feedstock plants	Advance integrated and consolidated bioprocessing with co-treatment	Generate drop-in biofuels (i.e., sustainable aviation fuel) and bioproducts from biomass and lignin residues
GLBRC	Conduct long-term studies of growing bioenergy crops on bioenergy lands	Design productive and high-value bioenergy cropping systems	Develop cost-effective biomass deconstruction and separation strategies	Identify and engineer novel biomass conversion microbes
JBEI	Design sustainable and cost-effective bioenergy cropping systems and conversion processes	Engineer bioenergy crops for high yield, environmental resilience, and efficient conversion into biofuels and bioproducts	Develop and demonstrate affordable feedstock-agnostic biomass deconstruction technologies based on ionic liquids	Develop high-throughput biosystems design tools and microbial hosts for scalable, carbon-efficient biofuels and bioproducts

CASE STUDY

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Advanced Bioenergy and Bioproducts Innovation (CABBI). The mission was defined by a new roadmap titled "Lignocellulosic Biomass for Advanced Biofuels and Bioproducts," which largely moved past cellulosic ethanol (U.S. DOE 2015b). Each BRC has developed a different strategy within the mission.

Several large-scale demonstrations have been discontinued for cellulosic ethanol biorefineries based on fermentation of agricultural residues with thermochemical pretreatment and added cellulolytic enzymes. However, the world continues to require sustainable biofuels to meet future energy demands based on climate projections (IPCC 2021; Junginger et al. 2019; Searle and Malins 2015). The BRCs target fundamental science with the mission of enabling sustainable bioenergy production while also modeling DOE science center management (Slater et al. 2015; Gilna et al. 2017; U.S. DOE 2018c).

The BRCs have excelled at driving domestic multidisciplinary, multi-institutional collaborations to solve common science problems, having produced more than 4,000 publications and impressive technology and intellectual property metrics since 2008 (see figure, Bioenergy Research Center Research Output, and table, Patents as Proxies for Innovation, next page). Such collaborations are often quite difficult to arrange on an *ad hoc* basis between independently funded principal investigators. BRC analyses demonstrate that many publications are collaborative, and CBI metrics suggest that increased collaboration is associated with publication in journals with high impact factors (see table, Example Publication Impact: Center for Bioenergy Innovation).

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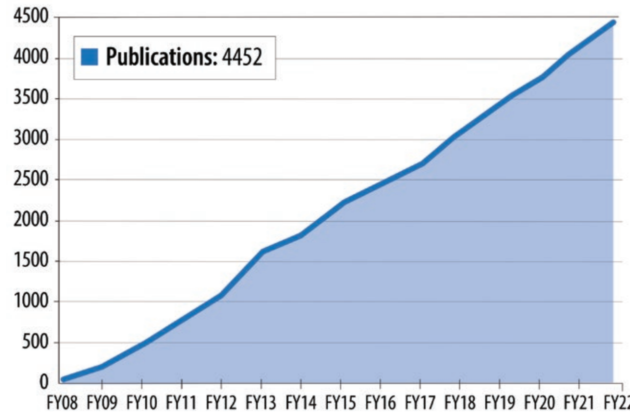
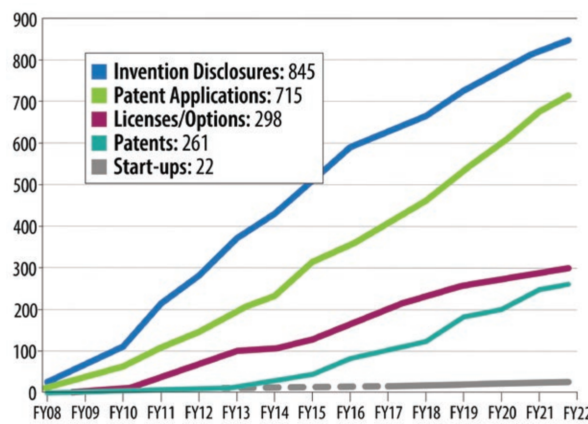




Bioenergy Research Center Research Output from 2008 to 2022. The figures illustrate cumulative publications for all four centers (top) and intellectual property (bottom).

Example Publication Impact: Center for Bioenergy Innovation*	
Publication Authorship	**Average Journal Impact Factor**
Single principal investigator (PI)	6.5
Multiple PIs	9.6
Single CBI partner	6.6
Multiple CBI partners	10.2
Combined multi-PI and multi-CBI partners	11.1

** CBI publications 2018 to 2021*

CASE STUDY

Continued from previous page

Despite this success, BRC research results have yet to experience major industrial deployments, possibly due to tension between long-term fundamental science goals and the near-term goals of the cellulosic biofuels and bioproducts industry, and the shift from cellulosic ethanol to alternative biomass-based advanced biofuels. One thought leader suggested that a more consortial approach with industry might alleviate this roadblock, although the intellectual property barriers might be high. Several precompetitive consortial models may be adaptable to this purpose, such as The National Institute for Innovation in Manufacturing Biopharmaceuticals and the Advanced Mammalian Biomanufacturing Innovation Center.

Patents as Proxies for Innovation

Agency*	Patents Per $100 Million Funded
DOE total	8
DOE Bioenergy Research Centers (2007 to 2021)	21
National Science Foundation	11
National Institutes of Health	5
U.S. Department of Agriculture	5
U.S. Department of Defense	2.5

** All agencies 2000 to 2013 except as noted. Source: NIH 2015.*

Continued from p. 15

et al. 2020; Woods et al. 2017; Huang et al. 2017; Liao et al. 2019).

- Democratization of the acquisition and analysis of plant and microbial metagenomics via JGI, a leader in these and other genomics-based achievements (Yang et al. 2017).
- Improved tools for genetic transformation in perennial feedstocks, nonmodel microorganisms such as bacteria or fungi with unique capabilities, and manipulated microbiomes, resulting in accelerated gene validation, metabolic engineering, synthetic biology, and model-guided metabolic redesign using, for example, KBase-hosted tools (Krause et al. 2018; Arkin et al. 2018; Chen et al. 2017; Mondo et al. 2017; Qiao et al. 2017; Xu, Q., et al. 2016; Ostrov et al. 2016).
- Evolution of genetic tool development for nonmodel organisms from an art to a method incorporating the latest gene- and genome-editing tools, including CRISPR/Cas9 for which BER-funded researcher Jennifer Doudna jointly earned the 2020 Nobel Prize in Chemistry (Bao et al. 2018; Haitjema et al. 2017; Shih et al. 2016; Xu, P., et al. 2016; Wannier et al. 2020; Lal et al. 2021; Riley and Guss 2021).
- Development and application of measurement, imaging, and modeling tools for massive genotype-by-environment phenotyping of plant feedstocks, plant-microbe interactions, and environmental microbiomes (Trigg et al. 2017; Ha et al. 2017; Abraham et al. 2016; Zeitoun et al. 2015; Kasanke et al. 2020; Lian et al. 2019); this work includes the (1) development of mass spectrometry imaging (e.g., secondary ion and nanostructure-initiator mass spectrometry) to elucidate biofilm-microbiome associations and individual molecular reactions and signals (Tetard et al. 2015; Victor et al. 2020; Velickovic et al. 2018; Kosina et al. 2021; Ding et al. 2021; Ing et al. 2021) and (2) achievement of the 2020 Gordon Bell Prize in supercomputing for the largest biodata network analysis ever performed.
- Evolution of microbiome science from descriptive to mechanistic and predictive (e.g., how plants

Box 2.1 Poplar Genome Sequence Sprouts Discoveries

Four decades after DOE identified the poplar tree as a potential bioenergy crop, scientists finished sequencing the *Populus trichocarpa* genome in an international effort led by the DOE Joint Genome Institute and Oak Ridge National Laboratory (Tuskan et al. 2006). Numerous new research directions and collaborations have since sprouted from that first tree genome. For example, mycorrhizal fungi genome sequencing has helped the research community understand how *Laccaria bicolor* influences poplar health (Martin et al. 2008) and how the most common tree root fungal symbiont *Cenococcum geophilum* helps plants adapt to drought conditions (Peter et al. 2016). By 2014, DOE researchers had sequenced 544 *P. trichocarpa* trees within its natural range from California to British Columbia to study its response to various environmental conditions including drought tolerance (Evans et al. 2014). Researchers at three of the four DOE Bioenergy Research Centers are now building upon the poplar reference genome to engineer strains with modified lignin to boost terpene production and improve the cost-efficiency of feedstock processing and conversion to biofuels (Bewg et al. 2022).

recruit beneficial microbes to resist pathogens) (Schulz et al. 2017; Xie et al. 2020; Albright et al. 2020; Zegeye et al. 2019), leading to insights in carbon and nitrogen cycling and drought resistance (Xu et al. 2018; Saifuddin et al. 2019; Levy et al. 2018; Raissig et al. 2017; Sebastian et al. 2016; Steidinger et al. 2019).

In addition to performing cutting-edge genome-based research, BER's success in bioenergy research is grounded in funding team-based and multi-institutional research groups and supporting longer-term projects, such as the BRCs, which are focused on solving real-world problems. Thought leaders noted that the BRCs have created scientist networks across the United States that successfully establish collaborations, introduce individual researchers to new techniques and instruments, and provide a community for post-doctoral training and career development (see Case Study: DOE Bioenergy Research Centers, p. 16).

BER has demonstrated international leadership in bioenergy research over the last decade, as represented by general citation-based trends (see Fig. 2.2, p. 20). BER-sponsored publications are more often cited than international publications and those from other U.S. funding programs.

However, BER may not maintain its historic and current bioenergy leadership in the future, as suggested by a downward trend in its percentage of highly cited publications over the last decade and a rising trend for international comparators. Thought leaders echoed the assessment that international research teams will soon match the quality and output of BER researchers.

This trend may reflect a fading bioenergy boom in the United States, but the destabilization of fuel prices by international political events also highlights U.S. economic vulnerability to disruptions in the global energy market and the critical need for a renaissance in bioenergy research. Indeed, in a March 2022 interview with CNBC's Andrew Ross Sorkin, Treasury Secretary Janet Yellen said, "Europe and the United States would be less exposed to the pressures that this conflict is putting on our energy markets if we had greater reliance on renewables." She emphasized that the United States needs "to move quickly to renewables that will give us a safer and more independent energy picture" (CNBC 2022).

As an international leader in bioenergy, BER is well positioned to usher in a revitalization that embraces innovative, high-risk/high-impact approaches for accelerating the attainment of bioenergy and soil carbon sequestration goals. High impact may depend on externalities beyond BER, such as agreed-upon

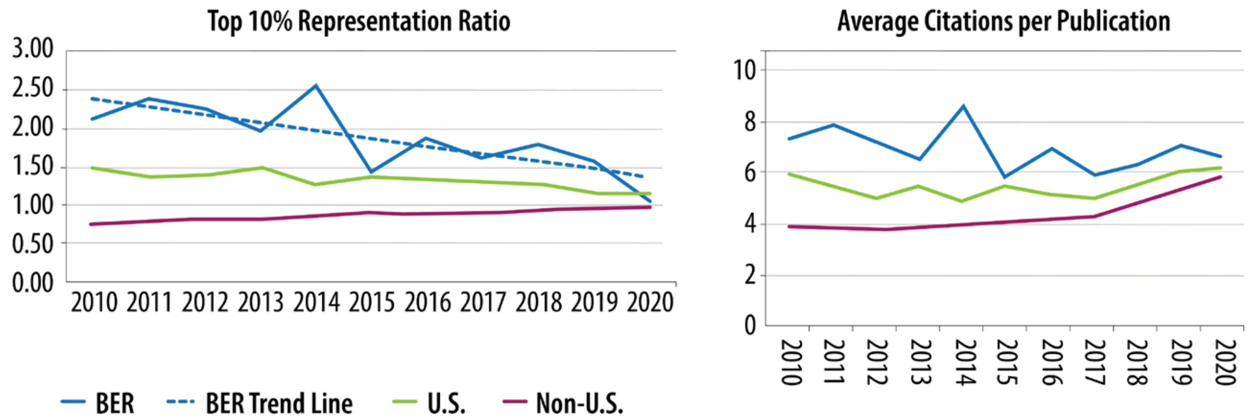


Fig. 2.2. Most Cited Bioenergy Research Publications. BER-supported bioenergy research publications have consistently outperformed publications sponsored by non-BER domestic and international funding programs. However, data over the last decade indicate a general downward trend in the number of top-performing BER publications and citations per publication. This decrease, along with rising trends among international comparators, suggests that the impact of BER research could soon be surpassed. The figure at left displays the ratio of a group's percentage of top-cited publications to its percentage of the total publication volume. Ratios greater than 1 indicate a disproportionately high representation among highly cited publications. [Courtesy DOE Office of Scientific and Technical Information]

measures of sustainability, policies that establish value for carbon efficiency and soil health, markets that return on these value incentives, and capital markets that favor lower capital and more rapid return on investment such as provided by IT sectors. Specific opportunities are discussed in Section 2.4, p. 26.

Plant Science

BER funding and studies in plant science have positioned the United States as the world leader in plant bioenergy and feedstock research. In the last decade, the United States published 60% of the publications in the field, which accounted for 40% of citations, followed by China with 13.5% and 9.7%, respectively.

BER currently supports several projects addressing challenges in plant science for bioenergy that fall under the themes of "Genomics-Enabled Plant Biology for Determination of Gene Function," "Systems Biology to Advance Sustainable Bioenergy Crop Development," and "Biosystems Design to Enable Next-Generation Biofuels." BER also supports the Plant-Microbe Interfaces SFA at Oak Ridge National Laboratory (ORNL) and the Quantitative Plant Science Initiative (QPSI) SFA at Brookhaven National Laboratory. Funded projects aim to (1) leverage omics-driven tools and systems biology to better understand the underlying genetic and physiological mechanisms influencing plant productivity, nutrient use efficiency, adaptation to abiotic stress, and beneficial plant-microbe associations and (2) validate functional roles for genes, gene families, and associated pathways in bioenergy crops (see Fig. 2.3, p. 21). This current research leverages "Plant Feedstock Genomics for Bioenergy" projects, which were part of a 12-year collaboration between BER and the National Institute of Food and Agriculture of the U.S. Department of Agriculture (USDA) aimed at accelerating plant breeding programs and improving biomass feedstocks. This example of interagency collaboration laid a secure foundation for genomics of dedicated bioenergy crops.

The United States holds a competitive advantage in sustainable bioenergy crop development because several countries view bioenergy crops as competition for land reserved for local commodity crops. BER is uniquely positioned to further transform the holistic understanding of bioenergy production by focusing on environmentally sustainable bioenergy crops that are robust producers on land not suitable for food crops

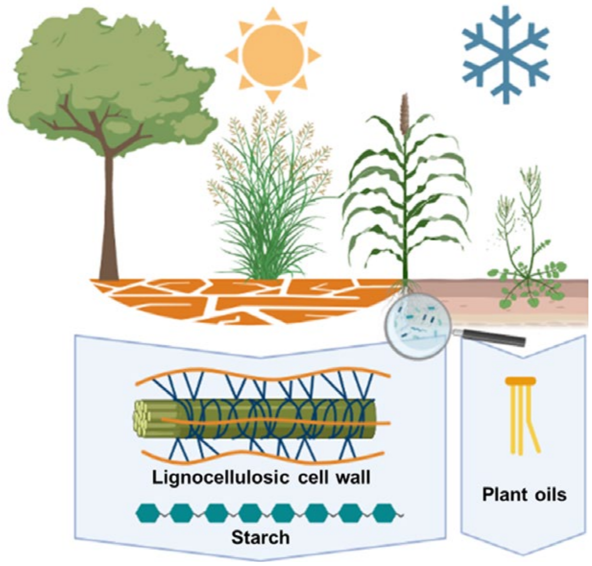


Fig. 2.3. Improving Bioenergy Feedstocks Through Systems Biology. BER leads in using systems biology approaches to understand energy-relevant plants and how the environment impacts bioenergy traits. [Courtesy University of North Texas]

and improving capabilities for understanding, predicting, and mitigating the impacts of energy production in a changing climate. Adding cover crops and perennials to priority bioenergy crops will help promote sustainable cropping systems. Some of BER's strengths and needs in sustainability research are outlined in the workshop report "Research for Sustainable Bioenergy: Linking Genomic and Ecosystem Sciences" (U.S. DOE 2014b).

Systems Biology

BSSD's support of systems biology approaches provides the necessary fundamental science to understand, predict, manipulate, and design biological systems. Systems biology, as first defined by Hiroaki Kitano, is the understanding of biology as a system of interacting parts (cells, tissues, whole organisms) with dynamic behavior that cannot be described simply as a sum of those parts (Kitano 2000). Systems biology research integrates molecular biology, genomics, functional genomics, and computational science. It represents the natural expansion of molecular biology with high-throughput genome-wide approaches born out of the revolutionary advancements in whole-genome sequencing (Westerhoff and Palsson 2004).

BER has stood at the forefront of genome biology research since its role in sequencing the human genome. This leadership has expanded into genomic investigations of DOE-relevant organisms using functional genomics approaches, metabolomics, proteomics, and genome-wide modeling. Predictive design is the ultimate expression of biological system knowledge and requires understanding not only molecular function but also biological networks and how network regulation translates into phenotype.

Through its scientific user facilities such as EMSL and JGI, BER's support for omics technique development and application (i.e., genomics, transcriptomics, proteomics, and metabolomics) has far-reaching impacts on many fields of study. DOE Early Career awardees view BER as the world leader in providing access to systems biology tools at user facilities and supporting high-quality omics-based publications.

2.2.2 Areas Requiring Strengthening

Thought leaders pointed to sustained funding as essential to reaching research goals and a major determinant in scientist recruitment and retention in bioenergy research. As the bioenergy boom faded in the 2010s, many early to mid-career researchers moved into biomedical research and pursued National Institutes of Health (NIH) funding. Retention is particularly poor in the fields of metabolic engineering, synthetic biology, "hard" (plant) biochemistry, physicochemistry, and scale-up. Thought leaders noted that few opportunities exist for early to mid-career national laboratory researchers to serve as principal investigators on BER research projects. Instead, these scientists serve supporting roles across multiple projects and must often significantly change their research focus to maintain support or realign their research activities to pursue non-DOE funding. These work arrangements have resulted in a reduced bioenergy workforce and potential loss of innovative scientists who could reshape bioenergy research with cutting-edge approaches.

In contrast to some international comparators, research funding in the United States is more stable due to the number and variety of agencies and programs. However, without coordination among funding agencies, research topics can become biased and siloed, resulting in overlooked bioenergy research areas, poor translation from basic research to scale-up and practical applications, and little to no collaboration among programs and agencies. Few opportunities exist for formal collaborations between basic and applied researchers.

To overcome the U.S. lag in transitioning science to biotechnological applications, BER should lead efforts to provide the fundamental knowledge needed to bring products to market. BERAC does not recommend that BER support applied research, since BER's strength and preeminence lie in fundamental science. However, BER should engage in creative opportunities to catalyze communication between basic and applied researchers to speed transition between early Technology Readiness Levels (TRLs), which are estimates of a technology's deployment maturity.

Thought leaders and early to mid-career scientists remarked that the United States is falling behind China and South Korea in industrial biotechnology and bioprocessing. Both countries excel at bench-to-product research and promoting successful collaborations between universities and industry. In South Korea, funding for bench-to-product research is perceived as easier to obtain than in the United States where funding sources must be pieced together.

Regarding workforce retention in bioenergy research, some thought leaders noted that although the United States trains many outstanding researchers, China attracts them with more research positions and funding. China has developed a focus on metabolic engineering and sustainable chemistry technology and hosts 4- to 5-fold more research groups in these areas than in the United States. Meanwhile, the United Kingdom leads in machine learning and artificial intelligence, largely due to the development of AlphaFold.

Plant Science

Thought leaders noted that U.S. expertise in plant biochemistry is fading as established leaders in the field begin to retire. Recognized rising stars primarily produce their cutting-edge research abroad. The paucity of biochemical characterization and functional enzymatic validation extends into microbiology as well, reflecting the rising dominance of computational, genomics, and functional genomics techniques that are less labor-intensive and generate more data than traditional biochemical approaches. However, the absence of biochemical characterization in plant sciences in particular erodes the potential knowledge that might be gained from genome-wide experiments. In addition, the lack of funding for molecular-level research has exacerbated the loss of data from genome-wide experiments as researchers and world-leading centers in the United States shift focus from plant science to medical research. The loss of research centers is particularly concerning because co-located researchers with complementary expertise and access to state-of-the-art equipment have been instrumental in innovation and discovery by serving as intellectual resources.

The thought leaders also noted large gaps between research communities performing basic research and applied research, such as plant cell wall biology and materials science. Investigations of biomolecular functionalities and physicochemical properties can inform the design of new plant-based materials with the potential to displace fossil fuels. Given this potential, research to characterize and exploit these new structure-function relationships is indispensable.

Systems Biology

Early Career awardees identified a need to support technology advancement and cutting-edge research to address weaknesses in data analysis and limitations in the types of omics data that are, or can be, combined for systems biology research. Balance also needs to be struck between computational predictions and ground truths to avoid systems biology and computational reconstructions becoming endpoints instead of engendering technological innovation when paired with molecular-level understanding and hypothesis testing. Finally, gaps exist between acquiring genome-based insights and translating that knowledge into sustainable bioenergy production, including linking systems biology to bioprocessing scale-up and scale-down.

2.3 Environmental Microbiomes Leadership Status

2.3.1 Overview

The GSP Environmental Microbiome research portfolio links the structure and function of microbial communities in the field with key environmental or ecosystem processes. Researchers apply systems biology, which couples modeling and theory, to define the organizing principles that control the functional capabilities of organisms. Studies range from plant-microbe interactions to *in situ* investigations of soil carbon and nutrient cycling to reduced-complexity model microbial systems at scales from molecules to landscapes. The research leverages multiomics, imaging, and computational approaches largely developed through BER-funded research.

Program Evolution

BER research in environmental microbiology originated with a major focus on contaminant cycling, including radioactive contaminants and mercury from DOE legacy sites established during the Manhattan Project and the Cold War. GSP continues to fund this research largely through the Ecosystems and Networks Integrated with Genes and Molecular Assemblies (ENIGMA) SFA.

Over the last decade, the focus and mission of GSP Environmental Microbiome research have shifted to climate change, carbon and nutrient cycling, and bioenergy feedstock sustainability. Increasing interest in soil carbon cycling, especially carbon capture and storage, reflects efforts to mitigate rising atmospheric carbon dioxide levels (see Fig. 2.4, p. 24). Other emphasis areas include the soil microbiome, plant-microbe interactions, and the development of environmental omics and data integration tools to study environmental microbiomes *in situ*. To differentiate itself from USDA soil microbiology research for agricultural crop production and from National Science Foundation biodiversity research, GSP focuses its soil microbiome science on bioenergy feedstock sustainability.

In its 2015 Strategic Plan, BSSD identified two systems biology–based focus areas for Environmental Microbiome research: (1) advancing sustainable bioenergy and (2) improving the understanding of carbon cycling and other biogeochemical processes (U.S. DOE 2015a). The plan described research needs related to plant-microbe interactions, including using microbes to deconstruct and convert biomass and improve sustainable biofuel systems in marginal soils under changing environmental conditions. The plan also outlined the need for research to predict the impacts of bioenergy cropping systems on belowground carbon capture and stabilization and to understand microbial roles in key biogeochemical cycles.

The 2021 BSSD Strategic Plan restructured the goals of GSP Environmental Microbiome research to focus on gaining "a predictive and functional understanding of microbiomes to better enable understanding of microbial ecology, plant-microbe interactions, and cycling of elements in terrestrial environments" (U.S. DOE 2021a). Although GSP currently supports limited research on methane consumption in marine sediments (Metcalfe et al. 2021), ocean research still lies outside its domain. However, coastal ecosystem projects are now included in BER's Earth and Environmental Systems Sciences Division.

Synergies and Current Projects

Today, Environmental Microbiome research is included in several major BSSD missions and research projects, including bioenergy and biodesign. Sustainable bioenergy objectives often complement those for environmental microbiome research in areas such as plant-microbe interactions, microbially mediated soil biogeochemical processes, and the impacts of both on sustainable bioenergy cropping systems. Complementarity also exists with environmental research projects supported through JGI's Community Science Program (CSP) and joint JGI-EMSL grants awarded through the Facilities Integrating Collaborations for User Science (FICUS) program.

GSP supports Environmental Microbiome science through national laboratory SFAs and university grants. In 2019, GSP awarded 10 university grants focused on systems biology–enabled research on the roles of microbiomes in nutrient cycling processes.

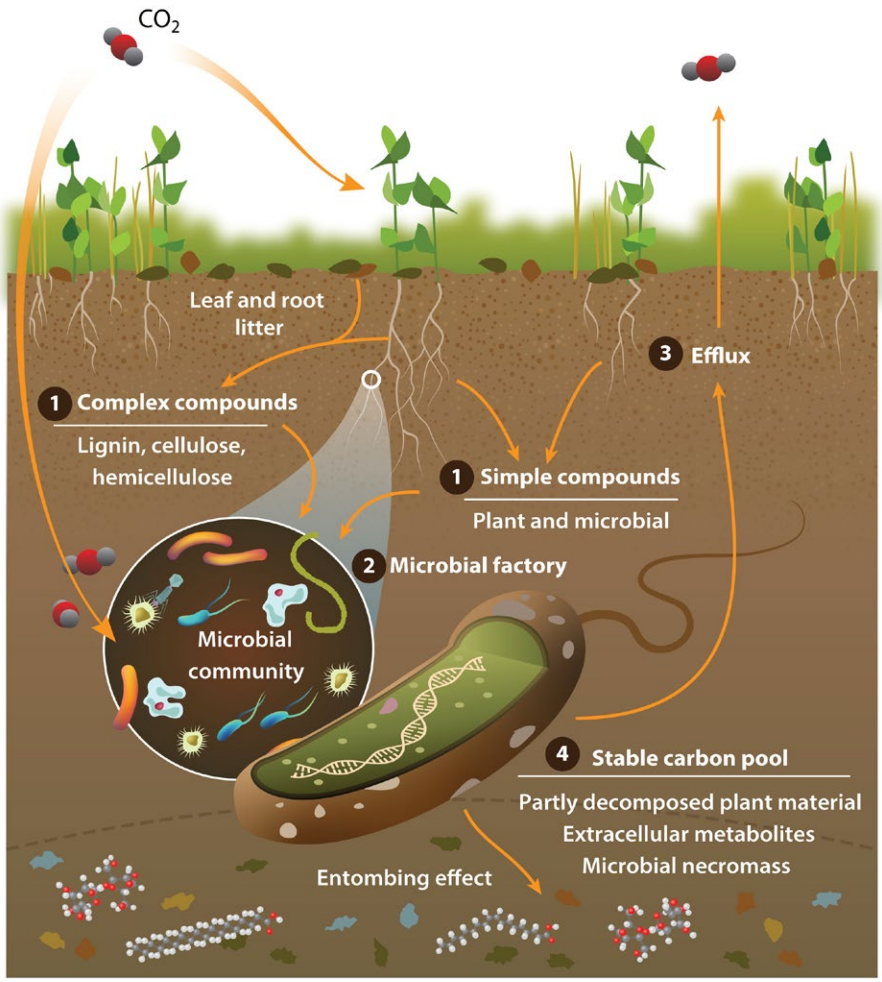


Fig. 2.4. Soil Carbon Cycling Through the Microbial Loop. Plants and autotrophic microorganisms fix atmospheric carbon dioxide (CO_2), adding it to soil where it becomes bioavailable to microbial metabolic "factories." [Reprinted under a Creative Commons Attribution 4.0 International License (CC By 4.0) from Naylor et al. 2020. "Soil Microbiomes Under Climate Change and Implications for Carbon Cycling," *Annual Review of Environment and Resources* **45**, 29–59.]

These projects seek to understand microbial responses to different environmental perturbations (e.g., drought, warming, and fire) and specific biogeochemical processes mediated by environmental microbiomes. At the national laboratories, SFAs in Environmental Microbiome science conduct research on bacterial-fungal interactions, the systems biology and phenotypic responses of soil microbiomes, plant-microbe interfaces, terrestrial microbial carbon cycling, and soil microbes used for carbon management and modeling. In addition, the Microbial Community Analysis and Functional Evaluation in Soils (m-CAFEs) SFA is developing a model system to study plant-microbe interactions (Zengler et al. 2019), and the ENIGMA SFA is studying processes affecting denitrification and metal reduction of nuclear materials within subsurface microbiomes at the DOE Oak Ridge Reservation in Tennessee. Three other national laboratory projects include two focused on engineering secure microbial systems—(1) Rapid Design and Engineering of Smart and Secure Microbiological Systems and (2) Intrinsic Control for Genome and Transcriptome Editing in Communities—and the Trial Ecosystems for the Advancement of Microbiome Science (TEAMS) project. Together, these projects advance omics, imaging techniques, and modeling approaches to study interactions among microorganisms, including inter-kingdom interactions among bacteria, archaea, viruses, fungi, and plants.

2.3.2 Successes and Impact

The United States is a world leader in environmental microbiome research, as evidenced by a literature search of *Proceedings of the National Academy of Sciences* and *mSystems* showing that 88% of publications containing the search term "environmental microbiome" originated in the United States. BSSD-funded science has leveraged considerable advances in genomics and other omics technologies to advance knowledge of environmental microbiomes (see Box 2.2, Pioneering Microbial Discovery from Environmental Microbiomes, this page). Similarly, Environmental Microbiome research has contributed to sustainable bioenergy objectives, such as understanding plant-microbe interactions and microbially mediated soil biogeochemical processes and their impacts on bioenergy crop sustainability.

BER support of JGI and EMSL user projects also has contributed to the success in Environmental Microbiome research. For example, cultivation of the *Populus trichocarpa* microbiome was funded through a CSP sequencing project at JGI. Direct funding to JGI supported several other noteworthy scientific achievements in environmental microbiology research outside of projects led by GSP SFAs or universities. For example, JGI metagenomics tools and resources recently enabled reconstruction of microbial genomes from environmental metagenome-assembled genomes (Nayfach et al. 2021) and retrieval of global environmental viral sequences (Paez-Espino et al. 2016). These achievements have provided a tremendous resource to the national and international scientific community by vastly expanding the known diversity of environmental microorganisms and viruses and by making the data publicly accessible.

Recent achievements in BER-funded Environmental Microbiome research include:

- Discovery of new anaerobic methane oxidation partnerships with nitrogen fixers (Metcalfe et al. 2021).
- Discovery of symbiotic partnerships between anaerobic methanotrophic archaea and sulfate-reducing bacteria that consume methane in deep-ocean methane seep ecosystems (Metcalfe et al. 2021).

Box 2.2 Pioneering Microbial Discovery from Environmental Microbiomes

Earth's microbes outnumber the stars in the Milky Way, but the vast majority remain uncharacterized because they are unculturable in a laboratory setting. In the last 2 decades, techniques such as single-cell genomics (jgi.doe.gov/jgi-at-25-a-single-cell-myriad-microbial-discoveries/) and metagenomics (jgi.doe.gov/from-life-at-extremes-to-editing-genomes-doudna-nobel/) pioneered and developed at the DOE Joint Genome Institute (JGI) have enabled researchers to extract genetic information from DNA samples from ecosystems around the world and reconstruct individual genomes, filling in nearly 30 major previously uncharted branches of the microbial tree of life (Hedlund et al. 2014; Rinke et al. 2013). More recently, data from more than 200 researchers around the world have contributed to expanding the known diversity of bacteria and archaea by 44% (Nayfach et al. 2021). Building from data derived from the first genomic characterization of a microbial community and from observations of CRISPRs in microbial sequences (Tyson et al. 2004), Jennifer Doudna and Emmanuelle Charpentier received the 2020 Nobel Prize in Chemistry for developing CRISPR/Cas genome-editing technology. Researchers continue to add to and mine the publicly available data on JGI's portals, particularly its Integrated Microbial Genomes and Microbiomes system, to find novel Cas genes and CRISPR systems (Harrington et al. 2018).

- Linkage of microbial degradation of *Sphagnum* moss in peat bogs to acetate mineralization using global insights and genome-centric analyses (St. James et al. 2021).
- Use of comparative genomics and metagenomic stable-isotope probing to characterize cellulolytic taxa that access carbon-13 from cellulose (Wilhelm et al. 2021).
- Development of new hypotheses and exploration of temperature sensitivity of soil processes in response to climate change (Alster et al. 2020).
- Discovery that evolutionary history exerts a stronger influence than environmental variation on differences in microbial growth and carbon assimilation rates between taxonomic groups (Morrissey et al. 2019).
- Development of a controllable soil environment for visualizing microbial community interactions (Bhattacharjee et al. 2020).
- Discovery of taxon-specific microbial responses to rewetting of a California grassland soil (Blazewicz et al. 2020), viral responses to soil wetting and drying (Wu et al. 2021a), and viral responses to historical moisture regimes (Wu et al. 2021b).
- Discovery that the availability of carbon sources influences the abundance of microbial taxa responsible for nitrate respiration (Carlson et al. 2020).
- Discovery that microbial diversity is important for carbon use efficiency in a model soil system (Domeignoz-Horta et al. 2020).
- Cultivation of *Populus* spp. root microbiomes (Carper et al. 2021).

2.3.3 Areas Requiring Strengthening

The United States has the expertise to explore and understand terrestrial microbial systems biology, plant-microbe interactions, and communities using high-throughput omics approaches. However, BER science could benefit from additional linkages to bioenergy sustainability research and efforts to increase soil carbon sequestration capacity in synergy with improvements to bioenergy feedstock crops. These linkages could occur through projects funded by the DOE Early Career Research Program, for example.

BER has supported pioneers in the field who have developed new methodologies and analytical techniques to evaluate complex microbial systems in soils. However, concern exists that BER will soon be eclipsed by countries with accelerating advancements in technology development and theory. The United States should strengthen international partnerships in the development of deep-learning techniques and the acquisition of training sets needed to better predict the functions of uncharacterized environmental molecules and proteins. The recent development of AlphaFold, a protein-structure modeling algorithm developed in the United Kingdom, highlights the potential for machine-learning techniques to revolutionize biology if large training sets are available (Jumper et al. 2021). The challenge for many researchers in the United States is rapid access to inexpensive and reproducible metagenomic sequencing data for use in computational models. Many core sequencing facilities in the United States are overwhelmed with demands and lack the staff to support user needs, whereas many companies in Asia provide fast sequencing data.

2.4 Future Opportunities

2.4.1 Crosscutting Opportunities

Crosscutting, multidisciplinary science and teams are a strength within BER. Nevertheless, opportunities exist for BER to support riskier but potentially “disruptive” science in the following ways.

- Provide infrastructure and funding mechanisms to help BER-funded researchers establish collaborations for testing hypotheses and characterizing candidate genes, proteins, and pathways resulting from BER-funded systems biology and computational biology research.
- Establish innovative forums that leverage video conferencing and in-person workshops combined with creative funding opportunities to encourage crosscutting, interdisciplinary research. To address the U.S. lag in transitioning its extensive

innovations in fundamental biological research to applications in biotechnology and industrial-scale outcomes, BERAC proposes implementing cross-program workshops between principal investigators funded from BER and other DOE programs, such as the Bioenergy Technologies Office. The resulting collaborative teams would seek to leverage the expertise of established principal investigators and the novel ideas of early to mid-career researchers to lower the intellectual and network barriers to achieving biotechnological applications of their fundamental research.

- Apply BRC-type research strategies and approaches to smaller team-based funding modalities led by universities and the national laboratories. This BRC approach could also be applied to related missions in soil carbon sequestration and biomaterials.
- Fund large-scale programs across DOE sectors focused on fundamental processes in environmental microbiome in key mission areas, such as developing sustainable bioenergy crops and understanding terrestrial cycling of carbon and other nutrients in the face of climate change. This effort would leverage the synergy between GSP Environmental Microbiome research and overlapping DOE research programs and sectors, including systems biology research, JGI direct-funded research, and environmental microbiology research supported by BER's Earth and Environmental Systems Sciences Division.

2.4.2 Bioenergy: Plant Science

Pressing challenges associated with global climate change can be addressed by understanding the carbon capture and conversion capabilities of plants in association with their microbial communities. BER research should endeavor to develop real-time evaluations of the physiology and metabolism of plants grown in the field with characterized microbiomes to build predictive models that integrate and represent multiple data types. One thought leader proposed that the "Holy Grail" is understanding how plants recruit microbes to the rhizosphere to suppress pathogens and aid resilience against biotic and abiotic stressors. The American Society of Plant Biologists affirms that, "plant and microbial genomics continue to be particularly ripe for exploration and progress." Similarly, BERAC encourages BER to expand its list of priority bioenergy crops to include additional cover crops and perennials that may promote sustainable cropping systems.

BER is a leader in generating high-quality genome-based resources and is therefore uniquely positioned to revolutionize post-genomic research that captures biological complexity and to develop approaches that address bottlenecks in data generation, analysis, interpretation, and translation. Toward these goals, an opportunity exists to upgrade field, greenhouse, and laboratory infrastructure to modernize data collection, support training across disciplines, and re-energize complementary biochemistry-based approaches for discovery-based research and ground-truth experimentation.

Efforts to innovate linkages between molecular and phenomic analyses can deepen the understanding of connections between plant-microbe community systems and plant physiology and productivity. The United States possesses the dedicated field facilities needed to grow commercial crops under production conditions, making this country the envy of international collaborators. Several thought leaders remarked on the easy access of field sites to researchers and the breadth of ongoing research that these sites support, which enables scientists to conduct experiments under real-world conditions and interact with biotechnology companies.

Opportunities exist for BER to increase leadership in the plant sciences by acknowledging the distinct life-cycle considerations of plant science projects, which require longer experimental times than other studies. A major bottleneck in studying plants is the time required to grow and generate stable, homozygous mutants. Three-year funding cycles are generally not sufficient to complete bioenergy crop studies. This challenge could be mitigated by providing opportunities to apply for additional or longer-term support (minimum 5 years) or to utilize established field trials within the BER programs.

2.4.3 Bioenergy: Systems Biology

BER is a recognized international leader in the systems biology of energy-relevant plants and microbes. To maintain this leadership, opportunities exist for BER to support technological innovations that not only describe system behavior but also better predict it (see Fig. 2.5, this page). Such innovation should integrate multiple omics experiments (such as genomics, transcriptomics, proteomics, epigenomics, metabolomics, and functional genomics) with synthetic biology approaches to achieve biosystems redesign with intended capabilities. Computational biology is a key component, but computational research should be paired with hypothesis testing based on experimental data. A key component to this strategy is integrating experimentation across scales, from molecules to phenotypes, and providing ground truths and genome-based principles that support accurate computational propagation of knowledge across diverse bioenergy-relevant genomes; a gap between biochemistry and functional validation was noted in Section 2.2.2, p. 21. BER supports bioenergy-relevant research that already has most of the necessary components, but integration is lacking. The program's portfolio also has the people and tools needed to form large-scale research teams that can help build a holistic, multiscale, predictive understanding of sustainable bioenergy cropping systems, their microbial communities, soil health, and ecosystem-level processes.

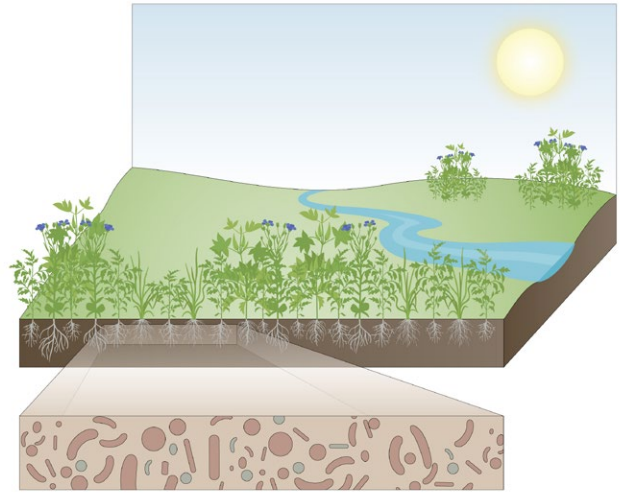
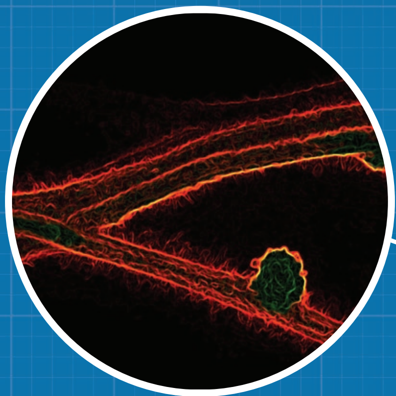
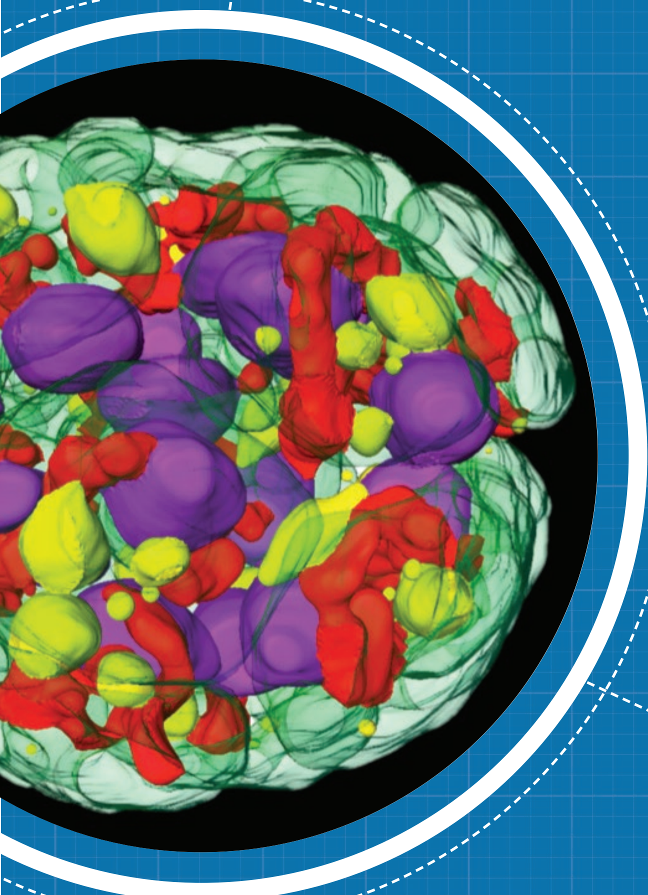


Fig. 2.5. Predicting Plant-Microbe Interactions. Systems biology approaches can be leveraged to gain predictive understanding of above- and belowground communities to achieve a sustainable bioeconomy. [Courtesy Lawrence Berkeley National Laboratory]

2.4.4 Environmental Microbiomes

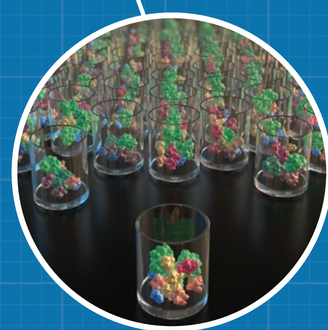
GSP has contributed significantly to understanding the tremendous diversity of Earth's microorganisms and viruses, with studies largely leveraging the high-throughput sequencing capabilities at JGI. However, most microbes in the biosphere have not been cultivated outside their native environments. Therefore, innovations in omics technologies, computational biology, and imaging are needed to better understand *in situ* microbial physiology and microbial interactions between plants and other microbes. An opportunity also exists to better harness the potential of soil microorganisms for carbon sequestration. These research opportunities require merging disparate expertise to answer key questions and bridging environmental microbiome and plant science research to innovate multipurpose carbon sequestration strategies that involve transforming CO_2 into bioproducts and stably storing CO_2 in soils.

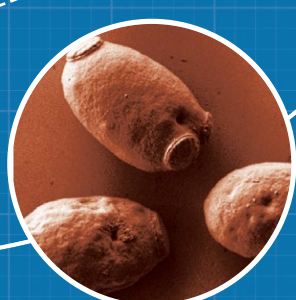




CHAPTER 3

Biosystems Design





Working Group Co-Leads

Himadri Pakrasi, *Washington University in St. Louis*
Kristala Prather, *Massachusetts Institute of Technology*
Huimin Zhao, *University of Illinois Urbana-Champaign*

Working Group Members

Nathan Hillson, *Lawrence Berkeley National Laboratory*
Costas Maranas, *The Pennsylvania State University*
Seung Yon (Sue) Rhee, *Carnegie Institution for Science*

Chapter 3

Key Findings and Recommendations

Key Findings

KF3.1 The relatively recent launch of BER's Biosystems Design research program is already yielding high-profile research accomplishments.

KF3.2 BER holds a strong leadership position in microbial biodesign, particularly in bacterial systems. However, leadership is increasingly distributed across the globe, with the United States considered "one of many" leaders for yeast and other fungi.

KF3.3 BER does not lead in understanding microbial physiology during bioprocess scale-up.

KF3.4 No world region yet leads in plant biodesign, suggesting that BER could target investments to yield substantial intellectual returns.

Recommendations

R3.1 Establish new Biodesign Research Centers patterned off existing DOE Bioenergy Research Centers to leverage advancements in BER's Biosystems Design research, which encompasses multiple applications and could potentially synergize various biological platforms, including non-model and photosynthetic microbes.

R3.2 Explore and coordinate joint funding calls with international agencies to accelerate progress in biodesign by leveraging key expertise from other countries.

R3.3 Encourage replication of recent machine-learning breakthroughs, such as AlphaFold 2.0, and development of new deep-learning algorithms more broadly in biodesign. Target funding for curating, mining, and generating omics datasets and developing laboratory automation tools for generating high-quality datasets to train machine-learning models that support biodesign.

R3.4 Invest in disruptive, bold initiatives to accelerate plant synthetic biology and plant transformation processes in coordination with the National Science Foundation and other agencies.

R3.5 Expand support for biomanufacturing training programs for doctorate and nondoctorate workforces that critically feed the talent pipeline for the U.S. biotechnology industry.

3 Biosystems Design

3.1 Overview of BER Biosystems Design Science

BER's 2 decades of pioneering support for biodesign science have made it the world leader in the field, as exemplified by its extensive supported research portfolio, the eminence of its supported researchers, and the quality and number of its publications. Within BER's Biological Systems Science Division (BSSD), biodesign lies at the core of the Genomic Science Program's (GSP) three primary research focus areas: Bioenergy, Environmental Microbiomes, and Biosystems Design. In general, biodesign involves biological systems engineering to achieve new or enhanced functions and traits beneficial for various applications. Design methods span evolutionary approaches that rely on generating and selecting or screening for improved variants to model-driven approaches that leverage either mechanistic or data-driven information to predict improved variants. Biological systems span the scale from single biomolecules (e.g., nucleic acids, proteins, or metabolites) to entire organisms (e.g., microbes, plants, or animals) to entire ecosystems composed of multiple interacting species (e.g., gut microbiomes, rhizosphere communities, or marine microbial communities) (see Fig. 3.1, this page).

Through its Bioenergy research program, GSP has invested in Bioenergy Research Centers (BRCs) that develop advanced biodesign tools for bioenergy and bioproduct production (see Case Study: DOE Bioenergy Research Centers, p. 16). Similarly, through its Biosystems Design program, GSP supports smaller projects and Science Focus Areas with multiple principal investigators who focus on developing new biodesign tools and capabilities. Examples include genome-scale microbial models; genome-scale engineering tools; bioproduction chassis; *in planta* production systems; and high-throughput and automated approaches for screening, characterization, phenotyping, and testing of engineered organisms.

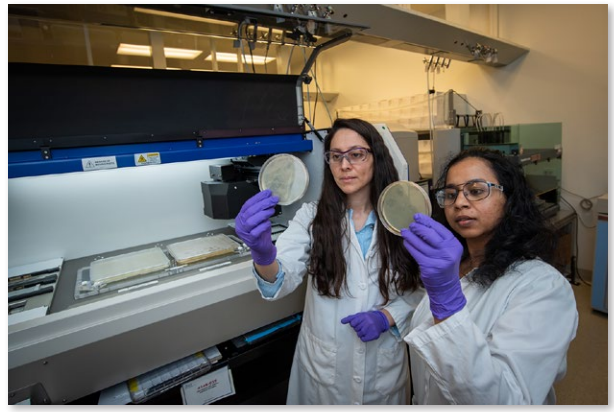


Fig. 3.1. A Crosscutting and Multiscale Approach. Biodesign lies at the core of the Genomic Science Program's three primary research focus areas: Bioenergy, Environmental Microbiomes, and Biosystems Design. Here, scientists examine microbial colonies on agar plates in front of an automated microbial transformation-plating and colony-picking robot (top). Plant scientists tend to tobacco plants, an important research tool for transient genetic transformation and protein expression (bottom). [Courtesy Lawrence Berkeley National Laboratory]

Critical to the future of the biodesign field, BER also supports various user facilities and the development of computational and instrumental platforms to enable broader integration and analysis of large-scale complex data within its multidisciplinary research efforts. Examples include the DOE Systems Biology Knowledgebase (KBase; kbase.us), National Microbiome

Data Collaborative (NMDC; microbiomedata.org), Structural Biology and Imaging Resources Portal (berstructuralbioportal.org), DOE Joint Genome Institute (JGI; jgi.doe.gov), and Environmental Molecular Sciences Laboratory (EMSL; www.emsl.pnnl.gov). Leveraging these ongoing research investments positions BER to continue leading the world in biodesign by integrating recent advances in data science (e.g., artificial intelligence and machine learning), genome-editing technologies (e.g., CRISPR), and analytical capabilities with its existing systems and synthetic biology capabilities.

3.2 BER's Biosystems Design Research Program

BER-supported biodesign research originated as an implicit part of the GSP portfolio, particularly within the BRCs. Ten years ago, however, BER created an explicit program in Biosystems Design within GSP with the objective to "advance fundamental understanding of genome biology and develop the genome-scale engineering technologies needed to design, build, and control plants and microbes for desired beneficial purposes" (genomicscience.energy.gov/biosystems-design/).

Biosystems Design research seeks to leverage the principles and practices of synthetic biology to enable rational, computer-aided design of biological systems to perform specified tasks. The program's objectives also emphasize automation and high-throughput analysis. Areas of interest include, but are not limited to, domestication of novel platform organisms with interesting phenotypes; genome engineering, including synthesis and delivery; cell-free systems; expanded understanding of sequence-function relationships at the genome level; biological synthesis and biodegradation of small molecules and macromolecules; and application of synthetic biology to consortia.

Only two DOE funding opportunity announcements (FOAs) have been issued and awarded for Biosystems Design, in 2012 and 2017, which precludes a meaningful statistical analysis of their outcomes. Therefore, BERAC provides here a qualitative assessment of these awards based on a review of the program's research portfolio.

The 2012 FOA covered two research areas: (1) microbial systems design for biofuels from computer modeling to experimental validation and (2) plant systems design for bioenergy. Four collaborative projects were funded within each area. This initial program yielded several highly cited papers, including one by King et al. (2016) reporting the development of a repository for more than 75 manually curated, genome-scale metabolic models. This publication exemplifies a tools-focused output that readily leverages the unique capabilities of DOE user facility systems such as KBase. It also indicates the emphasis of the Biosystems Design program on nonmodel organisms by including a broad range of biological organisms.

Two other highly cited manuscripts from Xu, P., et al. (2016) and Qiao et al. (2017) reported significant gains in understanding and engineering the nonmodel yeast *Yarrowia lipolytica* for the production of lipids and lipid-derived candidates for use as fuels and value-added chemicals. This work illustrates the impact of focused funding at a significant level to accelerate the translation of basic research from proof-of-concept to productivity metrics sufficient to generate commercial interest in an area important to BER.

This first FOA also generated highly cited papers for tool development in the area of plant systems design for bioenergy. Such tools and methods elucidate critical genomic and physiological features of plants and enable their rational design and engineering for user-defined purposes. In one example, Ming et al. (2015) sequenced the genomes of multiple pineapple species, with a focus on understanding the evolutionary origins of crassulacean acid metabolism, a water-efficient photosynthetic pathway for carbon dioxide fixation. Čermák et. al. (2017) also reported the development of a toolkit for genome engineering in plants based on TALENs and CRISPR/Cas9 and demonstrated its utility in five different plant species.

The 2017 FOA covered similar research areas: (1) integrating large-scale systems biology data to model, design, and engineer microbial systems for producing biofuels and bioproducts and (2) plant systems design for bioenergy. This round funded six projects within each area, with a mix of continuing and new principal investigators. Of the six microbial projects, five centered on nonmodel organisms with diverse feedstocks utilized for bioconversion, including carbon dioxide and lignin. The FOA explicitly noted cell-free approaches as an area of interest, with one of the projects using cell-free systems for rapid prototyping of system designs as the core of a *Clostridia* Biofoundry (DOE Assistance Award DE-SC0018249).

Projects that started under the 2012 FOA and continued into the 2017 FOA produced impressive demonstrations of high-throughput genome engineering and analysis. For example, manuscripts from the Ryan Gill and Huimin Zhao groups reported genome-scale tracking and engineering in *Escherichia coli* (Garst et al. 2017) and yeast (Bao et al. 2018; Lian et al. 2019), respectively. These papers describe essential technology required to facilitate biological design, particularly since predictive knowledge of genome structure and function is still lacking. The generation of large libraries can provide sufficient data to infer such relationships.

Although BER's Biosystems Design program is still young, it has already significantly affected the area of biodesign. By creating a distinct program, BER has accelerated development of tools and techniques that leverage existing systems biology infrastructure for biodesign and expand the application space to research areas squarely within BER's mission. To date, 20 funded research projects have yielded 380 peer-reviewed manuscripts, many of which are highly cited and leveraged by the scientific community. A notable success of the program is its development, or "domestication," of nonmodel microbes and plants. To achieve full deployment of these biological systems for biofuels and bioproducts production, and perhaps for the amelioration of environmental pollution, more platform organisms must be developed. This focal point has seen some success and is poised for even greater impact in the years ahead.

3.3 Leadership Status

3.3.1 Successes and Impact

To determine BER's standing in biodesign research relative to broader U.S. and international peer groups, BERAC undertook a bibliometric analysis. Biodesign research conducted in countries outside the United States, including Japan, Denmark, United Kingdom, China, South Korea, Australia, Singapore, France, and Germany, has produced significant advancements published in highly cited papers. Biodesign most closely associates with research categorized under the broad umbrella of synthetic biology, so BERAC chose search terms related to synthetic biology. Synthetic biology is a relatively young field, especially in comparison to other BER-relevant research areas. The bibliometric analysis was thus limited to an inclusive 10-year window (2010 to 2020) to understand BER's contributions compared to other U.S. and international researchers.

The analysis shows that U.S. researchers have consistently outpublished international researchers in terms of the number of highly cited manuscripts. Over the 10-year inclusive window, BER-supported biodesign publications comprised 2.3% of the total number of published manuscripts on average. When biodesign-relevant papers were ranked by number of citations, the representation of BER-supported publications rose to 5.9% of the top 1% ranked papers, 5.2% of the top 5%, 4.6% of the top 10%, and 4.1% of the top 20%. BER is correspondingly underrepresented in the lower tiers, comprising only 1% of the bottom 10% of cited publications (see Fig. 3.2, p. 34).

BER-supported leadership is especially evident in the early years of the analysis window, with an average of 11% of publications in the top 1% ranked papers for 2010, 2011, and 2012. In the later part of the decade, the data suggest that although the United States remains a leader in biodesign based on publication output, BER contributions decelerated slightly to track more closely with the national average. For example, over the last 3 years of the analysis window, BER-supported publications represent 4% of the top 1% ranked papers (see Fig. 3.2, p. 34). However, this does

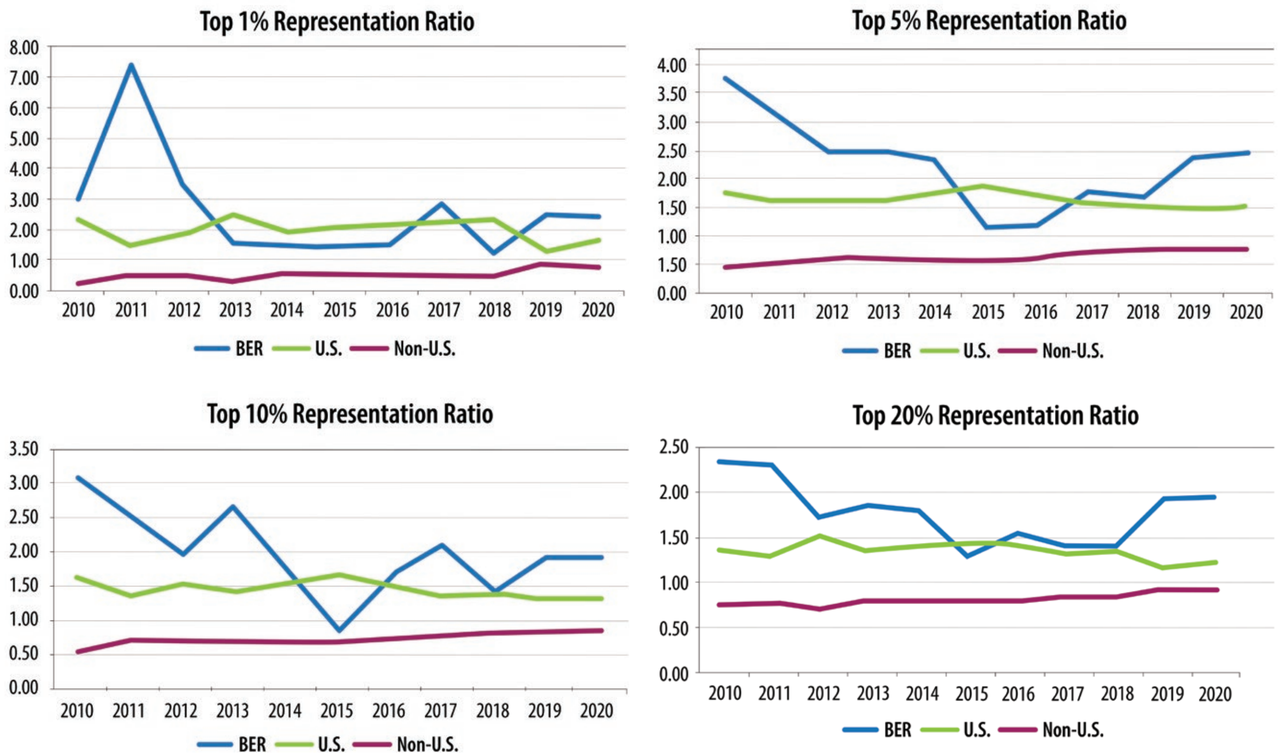


Fig. 3.2. BER Representation Among Top-Cited Biodesign Publications. The figures display ratios of a group's percentage of top-cited publications to its percentage of the total publication volume. Ratios greater than 1 indicate a disproportionately high representation among highly cited publications. [Courtesy DOE Office of Scientific and Technical Information]

not represent a decline in productivity, but rather is due largely to a few very highly cited papers in the early half of the decade.

Further analysis revealed that the most highly cited BER papers spanned methods and protocols, omics data resources for plant analyses, mixed microbial community analyses, novel biofuels, and novel synthetic biology devices. This suggests that BER's Biosystems Design research portfolio is intellectually diverse and impactful. For example, in 2011, BER experienced a 9-fold spike in its representation among the top 1% of cited biodesign papers, owing largely to a single manuscript cited nearly 1,000 times (Schellenberger et al. 2011). This protocols paper provided a definitive tutorial of the COBRA toolbox for constraint-based metabolic modeling and highlighted the importance of tool building and metabolic modeling to the broader scientific community. Two other 2011 manuscripts each garnered more than 350 citations (Sekhon et al. 2011; Peralta-Yahya et al. 2011). Sekhon et al. reported global transcriptomics profiles of maize across development stages and plant organs, providing broadly useful data on an important agricultural crop. This paper showcases the impact of plant omics resources in the broader scientific community. Peralta-Yahya et al. reported the microbial production of a plant terpenoid with properties comparable to diesel fuel by screening plant terpene synthases and optimizing the microbial chassis by metabolic engineering. Notably, these latter papers were published by two BRCs, exemplifying the value of the BRC funding modality in promoting biodesign research. In 2012, another paper reporting a genetic circuit that enables pathway-controlled dynamic regulation of metabolic flux garnered more than 500 citations (Zhang et al. 2012). This paper also

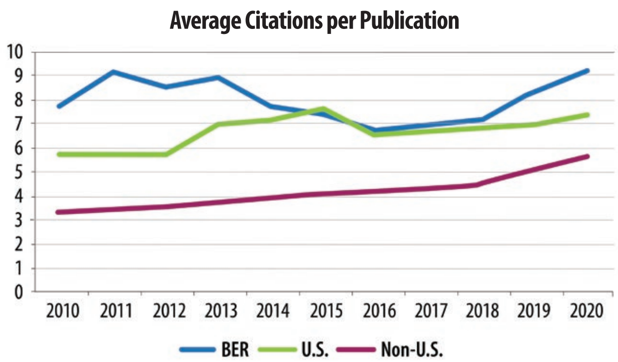


Fig. 3.3. Average Citations Per Biodesign Publication. BER has outpaced other U.S. and international research groups in terms of the 3-year rolling average number of citations received by its research publications. [Courtesy DOE Office of Scientific and Technical Information]

emerged from the BRCs and was the only biodesign-relevant manuscript with more than 300 citations that year. In 2015, the second-most highly cited paper in the 10-year period (>550 citations) reported the metagenomic analysis of an environmental microbial community (Brown et al. 2015). This work leveraged the capabilities of the national laboratories, including JGI's Community Science Program and EMSL.

An analysis of the average citations per manuscript during the 10-year window complements findings that BER and the United States can currently claim a leadership position in biodesign, but continued performance is not guaranteed (see Fig. 3.3, this page). BER's most highly cited papers were published between 2011 and 2015. The lag prior to 2011 isn't unexpected since citations are cumulative and may reflect the relative youth of synthetic biology (and biodesign) as a field prior to widespread growth. A regression of BER publications toward the U.S. mean starting in 2014 is correlated more strongly with an increase in citation rate among the full U.S. research cohort than a decrease in citation rate for BER-funded publications. It is worth noting, however, that the citation rate for non-U.S. contributions is slowly but steadily rising.

The international community generally perceives BER and the United States as leaders in designing microbial systems for sustainable bioproducts. However, leadership is becoming increasingly distributed around the world, especially in China with its rapid development of advanced capabilities.

Biodesign encompasses a broad range of research, from tool development to applications, and spans several biological platforms. With respect to leadership in specific biodesign-related areas, respondents perceived the United States as a leader in the design and development of tools and applications related to bacteria, whereas Europe and China excel at working with yeast and other fungi. The United States is viewed as only "one of many" in terms of understanding microbial physiology for fermentation, especially during scale-up, whereas China is building large and impressive facilities to accommodate bioprocess scale-up. The United States leads in engineering sustainable bioproducts, but China is poised to lead in engineering volume. The respondents predict that the United States and Europe will face strong competition from China on volume but may continue to lead in innovation. No country was perceived as a clear leader in plant biodesign research, suggesting an opportunity for BER.

In this context, BER constrains its leadership scope to the areas it chooses to fund. Because BER directs a significant portion of its budget to the BRCs, biodesign research largely comprises BRC research with a focus on a few microbial and plant systems rather than a more expansive approach. As a result, BER research is viewed as leading the development of application-specific tools but not necessarily the generation of general tools; this approach could put BER behind internationally if the application space pivots.

3.3.2 Commercialization

The United States leads in developing biodesign technology and transitioning it into the commercial space. This does not happen as efficiently in other parts of the world due to lack of access to capital markets and lack of business and legal frameworks. BER supports basic science research that facilitates the continuing emergence and growth of U.S. companies (see Case Study: From Biofuels to Bioeconomy—DOE Funding Helps Gingko Develop Leading Cell Programming Platform, p. 36), companies which do not have

Continued on p. 37

CASE STUDY

From Biofuels to Bioeconomy—DOE Funding Helps Gingko Develop Leading Cell Programming Platform

The early years of Ginkgo Bioworks were characterized by used laboratory equipment, low overhead, and exploration of different business models with the mission of making biology easier to engineer. The Boston synthetic biology company was founded in 2008 by four doctoral graduates and a professor from the Massachusetts Institute of Technology. Today, after receiving pivotal direct and indirect support from DOE, Ginkgo now boasts the leading platform for cell engineering, employs 700 people across five sites, and is publicly traded under the stock ticker DNA. The company delivers custom organisms that enable biotechnology applications across diverse markets, from food and agriculture to industrial chemicals and pharmaceuticals.

Long before Gingko attracted series A venture capital financing in 2015, the company received vital support from DOE in 2010 for a project called "Biofuels from *E. coli*" through the Advanced Research Projects Agency–Energy (ARPA-E) Electrofuels program. The project focused on engineering bacteria to use energy from electricity to fix carbon dioxide directly into biofuels with greater efficiency and cost effectiveness than biofuel conversion from biomass. For this project, Gingko collaborated with Jay Keasling at the University of California–Berkeley and David Baker and Mary Lidstrom at the University of Washington.

Through its support of training for core biotechnology skills and by facilitating advanced research, DOE has fostered a first-class bioeconomy workforce ready to contribute at Ginkgo and companies like it from day one. Dozens of Gingko's current employees have either conducted DOE-funded research, worked or interned at a national laboratory, or received a DOE fellowship during their training.

DOE is well-positioned to maintain its preeminent role in providing foundational support for the U.S. bioeconomy due to its ability to adapt funding and workforce training programs to reflect new capabilities needed for biotechnology applications that address some of the most pressing challenges. Like the ARPA-E Electrofuels program, much of the available funding for synthetic biology companies today goes to biofuels development. However, an important opportunity exists to leverage synthetic biology in other areas, such as climate change mitigation and prevention. For example, biomanufacturing is a highly efficient process that can often replace environmentally damaging extraction and synthesis processes across many sectors of the economy. A recent report from the McKinsey Global Institute estimated that up to 60% of the physical inputs to the global economy could be produced biologically, potentially reducing greenhouse gas emissions by 7 to 9% by 2040 to 2050 (Chui et al. 2020). DOE should continue to investigate its role in facilitating this economic transition and explore funding opportunities for bioeconomy start-ups to participate in realizing this opportunity.

Takeaway

DOE-funded workforce training outside of PhD tracks (e.g., associate degrees, apprenticeships, and certificates) is essential for the future bioeconomy.

DOE should likewise examine how its workforce development activities can be adapted for the modern bioeconomy. Historically, bioeconomy companies have required workforces with significant levels of higher education training, and DOE training support has mirrored this need. Today, however, the growing bioeconomy and increasing maturation of synthetic biology technology have shifted momentum to include workers who have completed associate degrees, certificates, and apprenticeship training programs. This welcome development not only drives the U.S. economy and international competitiveness but also promotes diversity, equity, and inclusion.

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traditional borders and may serve as effective bridges between nations.

An example of the impact of BER science on industry growth is the collaboration between LanzaTech, Northwestern University, and Oak Ridge National Laboratory. Supported by the Biosystems Design program, this collaboration is focused on developing a nonmodel acetogen for conversion of waste industrial gases to fuels and valued-added chemicals. The project leverages cell-free systems, which can be multiplexed for greater speed and throughput, to screen enzyme candidates and optimize their relative amounts. The experimental insights minimize the number of strains to be constructed and greatly reduce the time required for strain engineering (Karim et al. 2020). Recent results reported a strain producing acetone and isopropanol at very high rates (3 g/L-hr) and with high selectivity (90%) (Liew et al. 2022). LanzaTech recently announced plans to go public through a special purpose acquisition company merger valued at $2.2 billion (Ramkumar 2022). LanzaTech's success creates jobs in the United States and offers a means of using waste gases as feedstock for fuels and chemicals.

3.3.3 Supporting International Collaborations

Respondents emphasized the importance of promoting BER resources and facilities and improving outreach to the international biodesign community to maximize the impact of BER science. DOE can support international principal investigators, but such investigators often may not know whether they are eligible for direct grants, cooperative agreement funding, or user facility support. Respondents encouraged better coordination with other countries' funding agencies to leverage support for their portion of the collaboration. The National Science Foundation (NSF) has done this successfully.

Although different countries may not align on mission, they may align on basic science goals. BER could leverage these similarities to promote collaborations facilitated by entities like the Global Biofoundries Alliance (biofoundries.org), which already works with DOE-supported researchers. DOE could also follow NSF's example (Nikolaus et al. 2022) by encouraging U.S.-based scientists and engineers with active DOE awards, particularly those early in their careers, to pursue research collaborations with European colleagues supported through European Research Council grants.

The respondents also advise BER to coordinate efforts to collaboratively establish common standards, databases, and engineering methods. Some BER resources, such as KBase, appeal to international researchers but are infrequently used outside the United States. Similarly, principal investigators outside of the BRCs could benefit from improved access to high-throughput tools, but many are unaware of how to interact with entities like biofoundries.

3.4 Future Opportunities

3.4.1 Coordination with Other DOE and Federal Programs

BER's international leadership and future performance could be strengthened through better coordination with other DOE offices and U.S. federal agencies. For example, BER and DOE's Basic Energy Sciences program could work together to integrate biological and chemical catalysis. Recent effective interagency coordination efforts include collaborations between NSF investigators and the DOE Bioenergy Technologies Office (BETO) Agile BioFoundry (National Science Foundation 2022).

Respondents also encourage BER to form a stronger connection to DOE's Office of Energy Efficiency and Renewable Energy (EERE) to accelerate the translation of basic research to real-world applications, including process scale-up, especially given U.S. strength in launching start-ups. For example, BER could fund the first half of a 6-year grant and EERE the second half, to incorporate both basic and applied research activities into the same project. In addition, BER should develop connections with Advanced Research Projects Agency–Energy (ARPA-E).

In the context of workforce development, respondents suggested opportunities for DOE to partner with agencies such as the U.S. Department of Education and the U.S. Department of Commerce. This could involve regional partnerships between national laboratories and community colleges to train future operators and managers of facilities for jobs that do not require doctoral degrees (see Ch. 8: Strategies for People, Partnerships, and Productivity, p. 122).

3.4.2 New Biodesign Centers, Grant Supplements, and Demonstration Pilot Plants

Respondents noted that BER's focus on specific application areas may limit the overall impact of its supported research and, accordingly, U.S. potential to lead the field. One solution would be to develop biodesign centers styled after the BRCs, which have effectively catalyzed interdisciplinary, collaborative research in bioenergy. Biodesign centers would provide a similar framework for multi-institutional, multidisciplinary engagement toward tackling broader biodesign challenges.

BER also could offer grant supplements to cover emergent ideas that often develop during the initial phase of a research grant to help support U.S. innovation, creativity, and research agility. Early career scientists may find such mechanisms particularly useful as they transition into the next phases of their careers.

More demonstration pilot plants are needed in the United States, and DOE has a role to play (see Case Study: Amyris—Delivering on the Promise of Synthetic Biology, p. 39). Such facilities are key to international competitiveness and are also very relevant to workforce development to support an emerging bioeconomy. Many toll manufacturing options exist in Europe to help new companies launch production and sales, but little corresponding capacity exists in the United States. Achieving this type of infrastructure requires government support. Compared to the United States, Europe also appears to promote more academic-industrial partnerships to facilitate scale-up. BER could work toward this goal by strengthening its connection with EERE.

3.4.3 Plant Synthetic Biology and Transformation

A key development opportunity for BER leadership lies in plant synthetic biology. Advances and investments in genomics have produced a treasure trove of untapped information to understand basic principles of plant function and evolution and to develop applied solutions to national and global challenges. DOE's success in BER functional genomics and systems biology research and the ARPA-E Transportation Energy Resources from Renewable Agriculture (TERRA) program have identified candidate genes that impact biomass growth and resilience. Moreover, the demand for genetic transformation of plants has grown following breakthroughs in shoot regeneration via manipulation of developmental regulators and in genome editing via CRISPR techniques. The challenge now is to functionally validate candidate genes and generate edits that improve bioenergy crops through the design-build-test-learn cycle that is the hallmark of synthetic biology.

No world region yet holds clear leadership in terms of plant transformation and synthetic biology, according to BERAC's interviews with thought leaders, but a literature search for "plant transformation" and "plant synthetic biology" reveals that the United States leads in terms of publications (see Fig. 3.4, p. 41). However, China has been investing heavily into research and development, including synthetic biology, and in 2022 exceeded the United States in the number of publications on "plant transformation." China entered the field later than many other countries, yet its average number of citations per paper exceeds all other countries with higher publication rates, suggesting that China is increasing its production of high-impact papers (see Table 3.1, p. 42). Limiting the comparison of citation averages to 2017 to 2022, the United States drops from 25.1 to 8.1, suggesting declining competitiveness with other countries in plant synthetic biology. Now is the time for the nation to seize the opportunity to take a clear and profound leadership position in this space. The development of plant synthetic biology as a

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CASE STUDY

Amyris—Delivering on the Promise of Synthetic Biology

First Success

By the early 2000s, huge fluctuations in the supply and pricing of artemisinin, a drug used to treat malaria, had rendered antimalarial drugs expensive and inaccessible in many parts of the world, disproportionately impacting people in developing countries. In response, Jay Keasling, a professor of chemical engineering and bioengineering, and colleagues from the University of California–Berkeley launched Amyris in 2003 to synthetically produce artemisinin in greater quantities than it could be obtained from its original source—the *Artemisia annua* plant.

To address a global healthcare problem, Amyris pioneered genetic engineering and fermentation technologies to successfully produce artemisinic acid from yeast and sustainably sourced sugarcane. Pharmaceutical companies could then convert Amyris' artemisinic acid to artemisinin, making the entire process more efficient, reliable, and economical. The project was funded by a grant from the Bill and Melinda Gates Foundation, and Amyris went on to partner with the French pharmaceutical company Sanofi to license the artemisinic acid yeast strain and fermentation process on a royalty-free basis via OneWorld Health. In a first success, Amyris played an integral role in bringing millions of malaria treatments to people in need around the globe. The project set the tone for Amyris and its future endeavors to use synthetic biology to unlock innovative solutions to pressing global challenges.

Takeaway

Partnerships with R&D companies can amplify BER research impacts and bring BER-relevant processes to scale for market impact.

DOE Partnership

Following the successful artemisinin project, Amyris saw huge potential to apply the same underlying technology across other use cases, such as biofuels. This led to multiple partnerships between Amyris and DOE in which DOE provided funding to Amyris to explore using U.S.-based cellulosic feedstocks to domestically produce biofuels and sustainable products. Amyris has demonstrated the advantages and challenges of using cellulosic feedstocks for U.S. biomanufacturing, thereby opening new areas for research.

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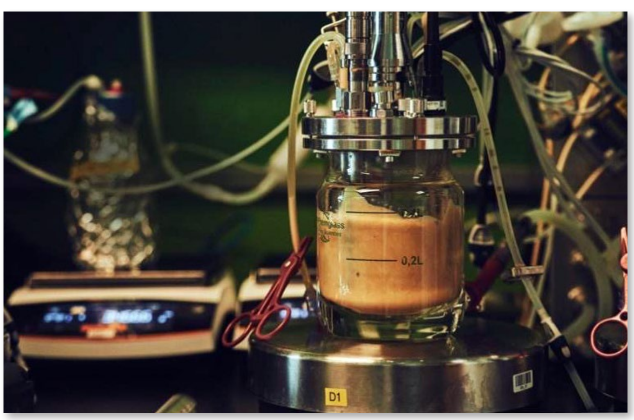

Putting Yeast to Work. Amyris scientists engineered yeast to produce artemisinic acid during fermentation (left), a chemical which is easily converted to artemisinin (right), a key ingredient in antimalarial drugs. [Courtesy Amyris, Inc.]

CASE STUDY

Continued from previous page

DOE funding enabled Amyris to bring new scale to its operations by investing in a state-of-the-art pilot plant facility at its U.S. headquarters in Emeryville, California. The pilot plant is a critical differentiator that enables Amyris to bring new products to market at unprecedented speed. Results of the partnership and funding have been especially beneficial at a time when the United States lacks sufficient pilot plant capacity; Amyris' in-house pilot plant has provided it with a competitive advantage in the industry.

Amyris also partners with DOE's Joint BioEnergy Institute (JBEI), a DOE Bioenergy Research Center established after Amyris' launch. JBEI research includes some of the most cutting-edge science and technology dedicated to developing independent energy supplies in the United States. Amyris' research and development leadership also plays active roles in several leading DOE-funded laboratories and centers, including the Agile BioFoundry, National Renewable Energy Laboratory, and Joint Genome Institute (JGI). Likewise, DOE-funded entities, including JBEI and JGI, support Amyris' talent pipeline as well as talent development for the entire biotech industry.

Beyond its partnership with DOE, Amyris has collaborated with other government agencies, highlighting the widespread impact that synthetic biology can deliver. Most notably, Amyris received funding from the Defense Advanced Research Projects Agency under the U.S. Department of Defense (DoD) to accelerate the design-build-test-learn cycle and develop scalable processes for producing novel molecules that are inaccessible through natural cultivation or other means. Multiple U.S. government entities are now testing some of these molecules for applications such as improving jet fuel performance and creating better flame-retardant materials. Amyris is also a member of BioMade, a DoD initiative to enhance domestic biomanufacturing capabilities.

Building a Sustainable Future

Amyris' go-to-market strategy has evolved over the years as market demands have shifted, but its vision has remained the same: harness the power of biology to build a sustainable future. To date, the company has commercialized 13 fermentation-derived ingredients found in more than 20,000 products that reach over 200 million consumers. Additionally, Amyris launched a family of nine consumer brands, all of which bring sustainable products directly to consumers through ecommerce and retail channels. With the foundational biotechnology platform that Amyris developed in the early 2000s, supported in part by DOE grants, the company has disrupted major markets and helped entire industries achieve new feats in sustainability with high-performing ingredients at scale.

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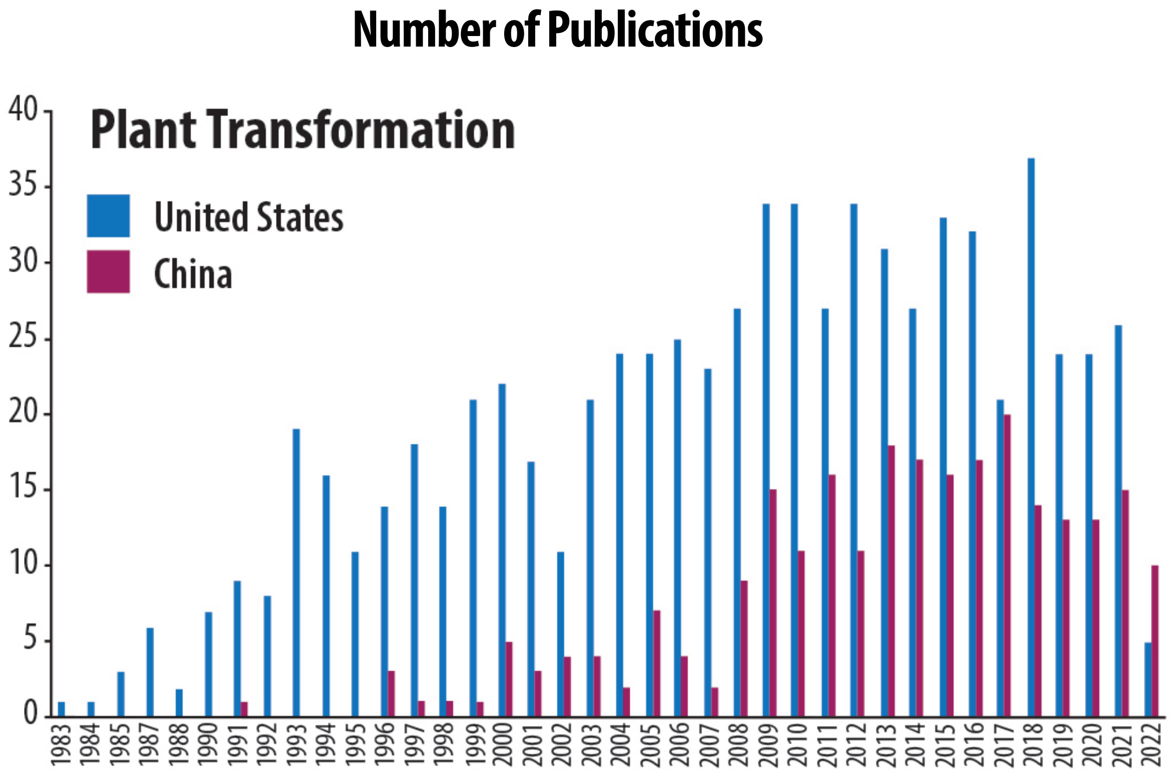
discipline with major potential impacts in biotechnology is a challenge that should be addressed at the scale of a BRC funding modality.

Overcoming Bottlenecks

The nation's ability to understand and harness the potential of plants is bottlenecked by (1) limited innovation in introducing and propagating foreign DNA in plants; (2) difficulty in accessing plant transformation technologies; and (3) immature capacities for modulating or reprogramming plant phenotypes. The United States acutely needs pioneering and innovative breakthroughs in the tools used to leverage plants to solve urgent problems, from energy to manufacturing. Partnerships across federal funding agencies and laboratories across academia and industry could enable widespread access and rapid translation of innovations and breakthroughs.

A dedicated facility or facilities would fill the dual role of providing plant transformation events to researchers nationwide while also producing breakthrough technologies in plant transformation. Including training



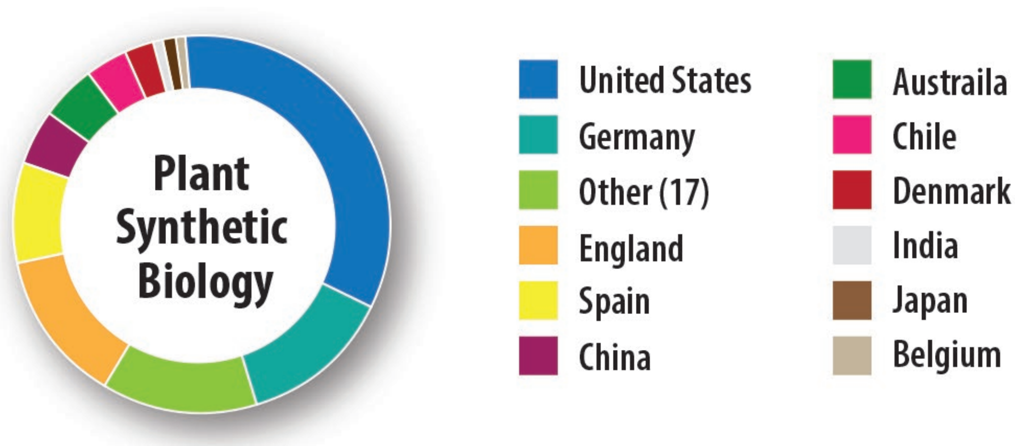


Fig. 3.4. United States Leads Publications on Plant Engineering. Published papers from the United States (blue) and China (magenta) retrieved with "plant transformation" as the search term (top) and proportion of papers published by different countries since 1900 with "plant synthetic biology" as the search term (bottom) using Web of Science on May 24, 2022.

Table 3.1 China Advancing with High-Impact Papers

Country	Total Publications	Citation Average	First Publication Year
United States	51	25.1	2008
England	22	36.36	2014
Germany	22	45.55	2012
Spain	17	49.82	2011
China	9	62.67	2017

Publication metrics from various countries with “plant synthetic biology” as a search term (Web of Science, June 6, 2022). [Courtesy DOE Office of Scientific and Technical Information]

as a substantive component would ensure that technology is translated to young scientists and individual laboratories. Currently, only a handful of laboratories perform robust transformation of bioenergy crops, so the development of training programs, visiting scholarships, and internship programs should be prioritized.

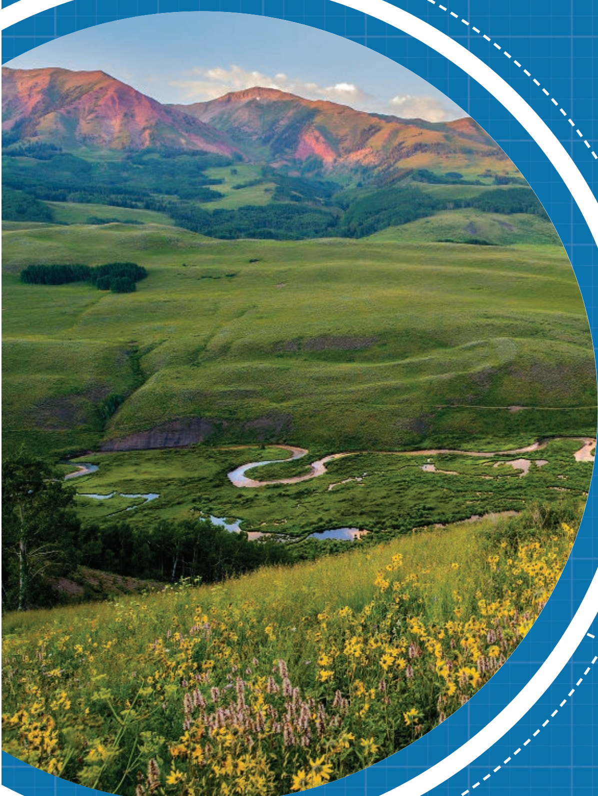
Funding and Infrastructure

To promote new horizons in transformation technology through visionary, high-risk, high-reward novel research, funding should be dispersed among targeted technology development groups as well as individual investigator grants. Equally important to funding centralized centers and facilities is support for individual scientists to test novel ideas, which may then feed into the creation of new facilities.

A dedicated facility or distributed network of facilities focused on high-throughput provision of transformed and edited plant material to DOE-funded scientists would dramatically improve research efficiency. High-throughput production of modified research materials in DOE focus species is optimally possible through integrated and uniform systems that take advantage of automation and information management systems. The expected annual output could reach thousands of constructs and tens to hundreds of thousands of events in a set of priority species and cultivars or taxa. Centers would link with current DOE facilities to use, for example, next-generation sequencing to characterize events and edits and to systematically gather expression, proteomic, and metabolomic data to support systems biology research projects. The centers would also coordinate regulatory and stewardship activities, perhaps including regulated field trial locations, to support use of materials by funded scientists.

CHAPTER 4

Environmental System Science



Working Group Co-Leads

Margaret S. Torn, *Lawrence Berkeley National Laboratory*
Michael N. Gooseff, *University of Colorado–Boulder*

Working Group Members

Efi Foufoula-Georgiou, *University of California–Irvine*
Markus Kleber, *Oregon State University*
Alistair Rogers, *Brookhaven National Laboratory*
Tim Scheibe, *Pacific Northwest National Laboratory*
Stan Wullschleger, *Oak Ridge National Laboratory*

Additional Contributor

Patrick Reed, *Cornell University*

Chapter 4
Key Findings and Recommendations

Key Findings

KF4.1 BER's Environmental System Science (ESS) research program is highly cited and internationally respected for its:

- **a.** Multidisciplinary systems science.
- **b.** ModEx (modeling-experimental) approach that emphasizes an iterative exchange of knowledge and discovery among predictive models, experiments, and observational field research, leading to novel discoveries, as demonstrated by, for example, the Next-Generation Ecosystem Experiments (NGEEs).
- **c.** Research infrastructure, including large-scale ecosystem manipulations such as the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project, AmeriFlux, and watershed Science Focus Areas, which support cross-agency and international collaboration.
- **d.** Terrestrial Ecology research, including biogeochemistry, ecosystem fluxes, and climate change responses.
- **e.** Watershed Sciences research, including multiscale hydro-biogeochemical modeling and process studies.

KF4.2 ESS research has untapped potential for:

- **a.** Better integrating human influence into the study of natural systems.
- **b.** Supporting both creative discovery science and the translation of research to inform applied solutions.
- **c.** Bridging the gaps between terrestrial sciences and atmospheric and climate sciences.

Recommendations

R4.1 Embrace coupled human-natural systems as a critical niche for ESS contributions in the next decade while maintaining the focus on mechanisms and process understanding.

R4.2 Elevate and integrate tools for data discovery and analysis at a level commensurate with ESS data volume and complexity to accelerate scientific impact.

R4.3 Facilitate the translation of ESS research into solutions and innovations by the DOE offices with a mandate for applied work and other potential partners.

R4.4 Create avenues for the research community to communicate and interact across the DOE science and technology pipeline, leading to breakthroughs, greater inclusivity, improved efficiencies, and reduced time lags between needs assessment, fundamental science, and application.

R4.5 Become an international leader in providing safe and inclusive fieldwork by building on existing ESS accomplishments, developing and sharing ESS resources, and modeling the successes that arise from equitable professional environments.

R4.6 Maintain global leadership in large-scale ecosystem manipulation experiments, a hallmark of BER science, which integrate ESS domains, promote ModEx, and foster collaboration among domestic and international institutions.

R4.7 Ensure that ESS strategic priority and funding paradigms support foundational research opportunities to continue international domain leadership.

4 Environmental System Science

4.1 Overview of BER Environmental System Science

BER's Environmental System Science (ESS) program targets Terrestrial Ecology, Watershed Sciences, and Coastal Systems (see Fig. 4.1, this page), which often are insufficiently represented in process models and multiscale Earth system models (ESMs). ESS seeks to fill significant knowledge gaps in current and predictive understanding of these systems, helping to provide a scientific foundation for solutions to DOE's most pressing energy and environmental challenges. Many ESS observations and modeling efforts are shaped by or used in other BER research activities such as climate science (see Ch. 5, p. 63), facilities and infrastructure (see Ch. 6, p. 83), and integrative science (see Ch. 7, p. 103).

ESS Terrestrial Ecology research seeks to improve the representation of terrestrial ecosystem processes in ESMs, thereby enhancing the robustness of model projections of how these ecosystems will respond to and impact a changing climate (ess.science.energy.gov/terrestrial-ecology/). Terrestrial Ecology research focuses on understanding ecosystem responses to warming temperatures, rising atmospheric carbon dioxide (CO_2) concentrations, changes in nutrient cycling, and altered precipitation timing and amount. Such understanding is essential to improving predictions of both the ecological effects of climate change and feedbacks between terrestrial ecosystems and the rest of the Earth system.

Watershed Sciences research seeks to advance a robust, predictive understanding of how watersheds function as integrated hydro-biogeochemical systems and how these systems respond to disturbances (ess.science.energy.gov/watershed/). Disturbances of interest include changes in water recharge, availability, and quantity; nutrient loading; wildfire; land use; and vegetative cover. ESS emphasizes a systems approach to probe the multiscale structure and functioning of watersheds and to represent the terrestrial subsurface and ecohydrological interactions in mechanistic models ranging from microbial metabolic processes to biotic-abiotic interactions to system responses at multiple spatial and temporal scales. ESS supports a network of watershed testbeds in diverse physiographic regimes for integrated field research and numerical modeling by national laboratory–led Science Focus Area (SFA) projects, university-led projects, and community collaborators.

Coastal Systems research, a new focal domain for BER, seeks to enhance basic knowledge and address uncertainties in the prediction of integrated coastal environmental systems and to improve their representation in ESMs (ess.science.energy.gov/coastal/). The

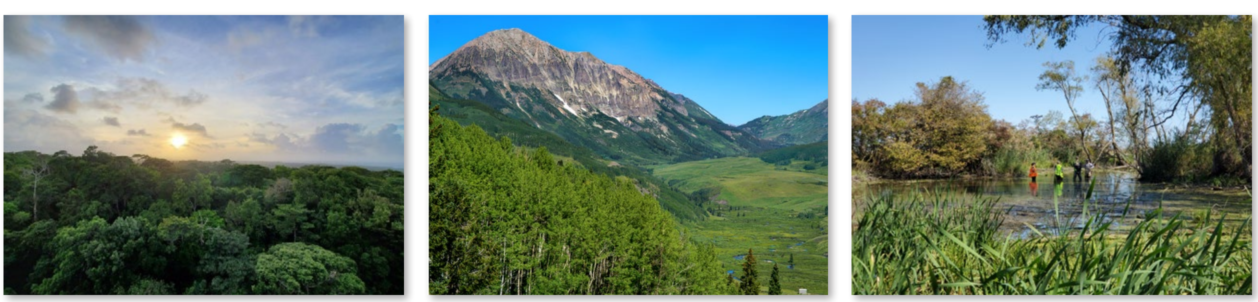


Fig. 4.1. Collaborating Across Environmental Science Domains. Terrestrial Ecology, Watershed Sciences, and Coastal Systems make up the three domains of the BER Environmental System Science program. [Courtesy Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Pacific Northwest National Laboratory]

complexity of coastal processes demands research that brings together a broad range of capabilities and tools and advances models, experiments, and observations across scales. This kind of multiscale system science builds on BER strengths and fits well with ESS strategic goals. BER also sees an opportunity to apply new variable-resolution capabilities in DOE's Energy Exascale Earth System Model (E3SM) and process models to represent the coastal land-water interface and its dynamic processes and drivers.

Globally, the environmental science community performs research on additional topics related to resource management, including research to (1) quantify or enhance terrestrial carbon sequestration, (2) manage groundwater and watersheds to ensure sufficient drinking water quality and quantity, (3) restore aquatic habitats, and (4) understand coastal systems adaptation to climate change. The DOE Office of Science does not currently pursue leadership in these areas, but future opportunities for BER may exist in these domains.

ESS funding for long-term projects, such as SFAs and Next-Generation Ecosystem Experiments (NGEEs), has been relatively stable across funding cycles, but annual variability in the overall ESS budget has been substantial. Between fiscal year (FY) 2010 and FY 2020, ESS annual funding averaged $73 million, declining by as much as 12% and increasing by as much as 27% during the decade. Funding reached a low of $53 million in FY 2017 and a high of $83 million in FY 2020. (This summary of funding trends is reported in 2010 dollars.) In addition, DOE historically has issued few competed funding opportunity announcements (FOAs) that cross programs, agencies, or divisions.

4.2 Leadership Status

To assess ESS's international standing, BERAC's Environmental System Science Working Group performed quantitative analysis of publication metrics and gathered input from thought leaders and scientists from all three ESS topical domains as the primary means of evaluation. Based on these assessments, BER is recognized as a leader in multiple areas of environmental system science.

Thought leaders represented various institutions and countries and a range of career stages. Of the 18 interviewees and 10 respondents to a federal Request For Information (RFI), 13 were academics and 15 were federal or foreign scientists or agency managers; 25 were in the United States and 3 were at foreign institutions; 7 were at early career stages, 6 were mid-career, and 15 were advanced career. Competitor institutions included Earth system science laboratories supported by the National Science Foundation (NSF), the National Oceanic and Atmospheric Administration (NOAA), and other agencies and major U.S. universities. International competitor institutions included the Max Planck Institutes and non-U.S. universities.

This section presents results of the publication analyses, describes topics and modes of successful leadership identified by respondents, and discusses areas where BER might enhance its standing and impact.

4.2.1 Publications

From 2010 to 2020, BER invested $805 million in the ESS program, not including user facilities. This BER support was credited in more than 1,700 peer-reviewed environmental science articles over this period, which were identified using ESS-related search terms listed in Appendix C: Approach to Metrics and Methodologies (see p. 151). The search terms generated an incomplete yet unbiased set of publications and citations for comparing BER and non-BER publication metrics. The analysis shows that BER-supported peer-reviewed publications in ESS domains are well cited and have produced an outsized scientific impact compared with non-BER papers.

While BER's 1,700 publications comprise only 1% of all publications with ESS keywords in this analysis, papers based on BER research have large scientific impact in terms of citations or other leadership metrics. For example, BER publications averaged more citations than non-BER U.S. and international publications (see Fig. 4.2, p. 47), and they contributed a disproportionately large number of the top-cited papers.

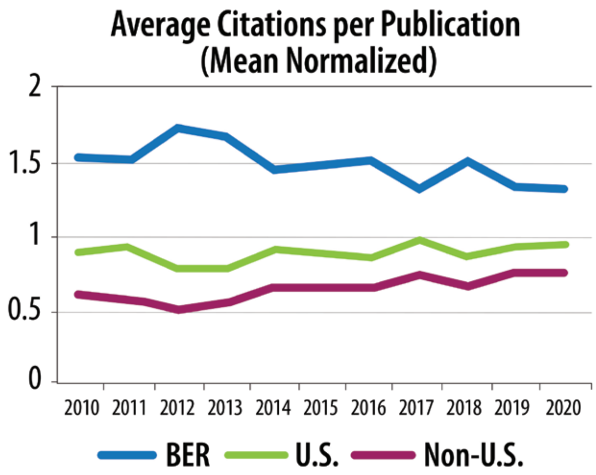


Fig. 4.2. Average Citations of Environmental System Science Publications. The plot shows the ratio of average citations per publication for BER-supported research divided by average citations for non-BER papers. Use of a ratio normalizes the number of citations over time. [Courtesy DOE Office of Science and Technical Information]

Specifically, the number of BER publications among the top 1% of most highly cited papers was on average more than five times the share of international papers and more than nine times the share of all U.S. papers (see Fig. 4.3, p. 48).

4.2.2 ESS Domain Leadership

Interdisciplinary, multidomain science is a hallmark of the three ESS thematic areas: Terrestrial Ecology, Watershed Sciences, and Coastal Systems. Watershed Sciences, for example, brings together hydrologists, geologists, biogeochemists, and ecologists to study the complex interrelated functions of these natural systems. This interdisciplinary approach is facilitated by DOE's science model, which supports the agency's mission without a structure that siloes different disciplines, as is done by NSF, the U.S. Department of Agriculture (USDA), and NASA. Within DOE's interdisciplinary framework, however, several respondents noted a shortcoming: human-natural system interactions are not well considered in BER-sponsored studies and, consequently, in the program's broader scientific vision and mission. This gap is a significant omission from modern environmental research, given the pervasive influence of humans on natural systems globally during the Anthropocene Epoch.

One significant strength of BER science is its rich history of scientific discovery and innovation through modeling. The ESS community develops and uses conceptual and numerical models that serve as integrating research frameworks. Some respondents recognized this as a product of the ModEx effort, in which researchers use models to integrate system insights and then to identify knowledge gaps and methodological challenges in understanding system dynamics. This iterative modeling-experimental cycle promotes new studies to improve both fundamental process understanding and model representations (see Fig. 4.4, p. 49).

Another distinguishing characteristic of the ESS portfolio is its large-scale, long-term, and interdisciplinary projects, such as SFAs and NGEEs, including manipulation experiments like Spruce and Peatland Responses Under Changing Environments (SPRUCE, mnspruce.ornl.gov). These projects leverage experts from multiple disciplines, including modelers and experimentalists, and address science questions too complex for individual investigators to tackle. Notably, they focus on scientific grand challenges and are funded on decadal time scales, enabling more integrative research that can evolve as system understanding is refined over time through observations, experiments, and conceptual and numerical modeling. Several respondents also noted that such projects take advantage of DOE national laboratory strengths in facilities, novel instrumentation, and modeling. Funding for these projects has enabled scientists to develop new research approaches and platforms, including community testbeds for Watershed Sciences and Free-Air CO_2 Enrichment (FACE) experiments for Terrestrial Ecology (U.S. DOE 2020b). Respondents describe such platforms as ambitious, sophisticated, and well beyond what academic investigators could undertake alone. Moreover, respondents view SFAs and NGEEs as exemplary investments that integrate sustained novel observational campaigns with advanced modeling to develop insight and foresight into Earth system processes. These strengths are

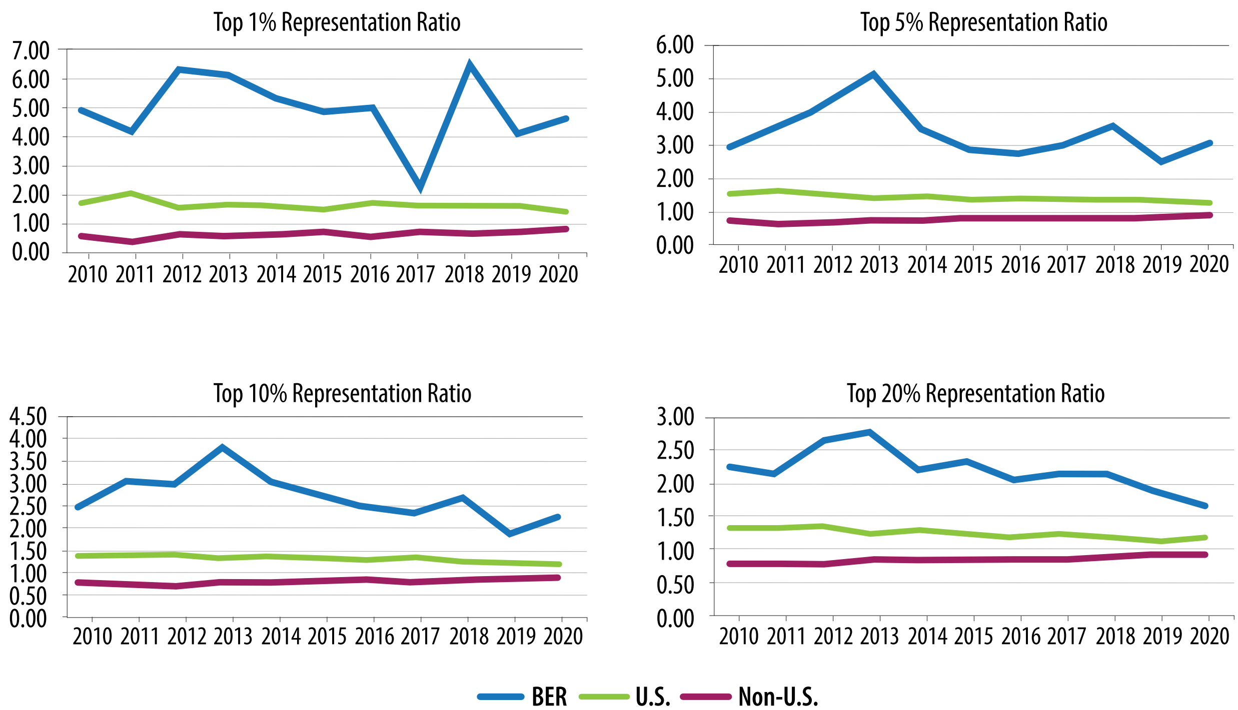


Fig. 4.3. Authorship of Environmental System Science Publications in the Top Citation Percentiles. The plots show the proportion (Y axis) of BER, other U.S., and non-U.S. publications that achieved the top 1st, 5th, 10th, and 20th percentiles for citations. The higher percentage of BER publications in top percentiles indicates higher impact and higher value per unit of publication. The figures display ratios of a group's percentage of top-cited publications to its percentage of the total publication volume. Ratios greater than 1 indicate a disproportionately high representation among highly cited publications. [Courtesy DOE Office of Science and Technical Information]

coupled with the development of new technologies and applied to research missions across the BER portfolio.

The BER research community's participation in strategic planning workshops and high-profile scientific reports extends the impact of BER science nationally and internationally and demonstrates the leadership of BER-supported scientists. For example, ESS research directions are shaped by BER-supported community-led workshops whose outputs are captured in various BER and BERAC Grand Challenge reports (ess.science.energy.gov/pubs). These documents tie new BER initiatives, such as the NGEEs and terrestrial-aquatic interface science, to robust scientific priorities and state-of-the-art approaches. In addition, BER scientists contribute to many high-profile reports, such as the U.S. Global Change Research Program's State of the Carbon Cycle Reports and National Climate Assessments; Intergovernmental Panel on Climate Change assessment reports; and National Academies of Sciences, Engineering, and Medicine documents.

4.2.3 Terrestrial Ecology

Respondents recognized BER Terrestrial Ecology science for its successful leadership in four main categories: research topical areas, large-scale ecosystem experiments and integrative research, ModEx, and model development and use.

Research Topical Areas

BER advances U.S. leadership in (1) soil biogeochemistry, (2) terrestrial ecosystem ecology and fluxes, (3) climate change impacts and responses,

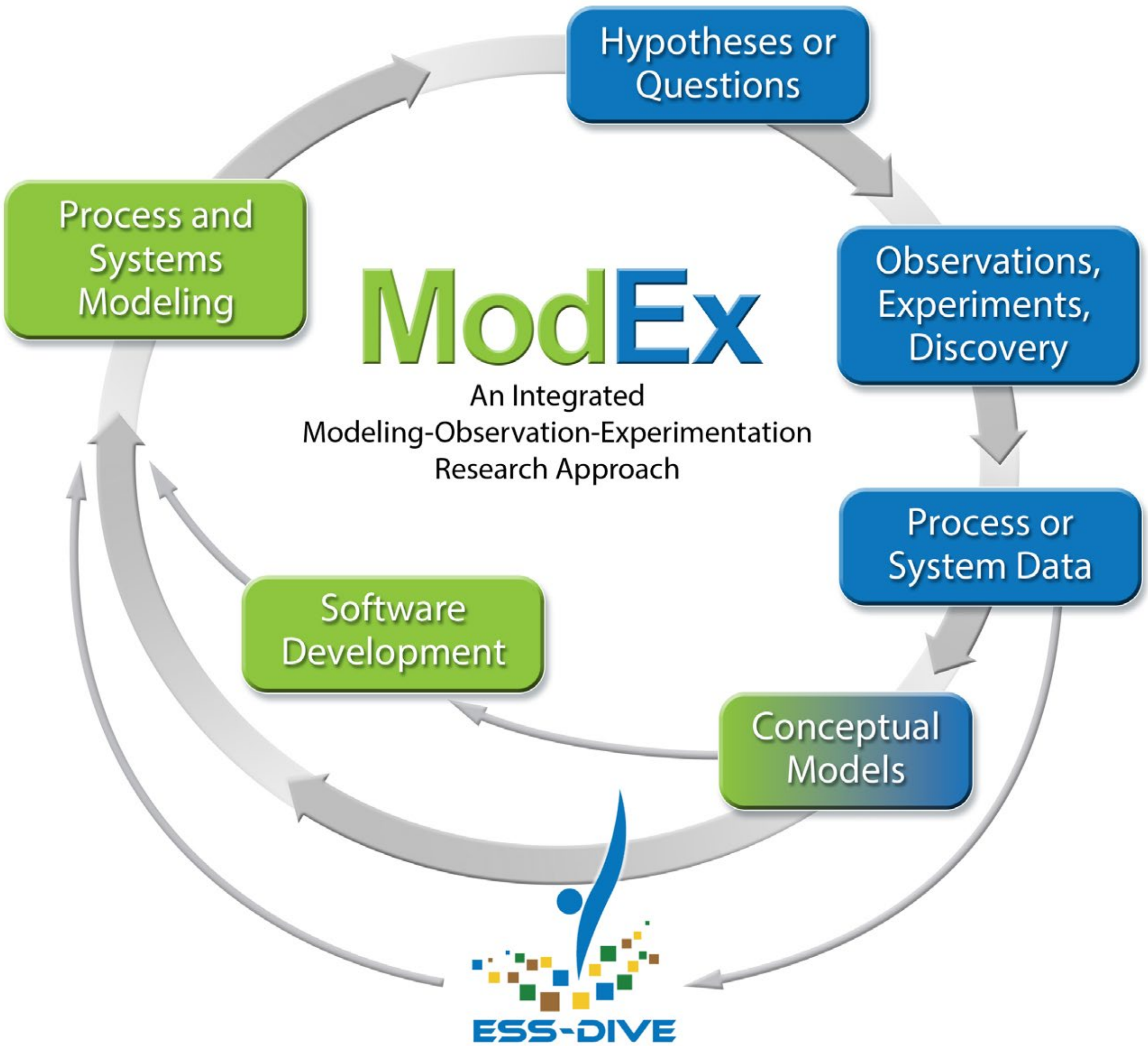


Fig. 4.4. BER's ModEx Approach: Integrating Modeling, Observations, and Experiments. Within the ModEx framework, researchers combine process research (including observations, experiments, and measurements performed in the field or laboratory) with modeling activities that simulate these same processes. This integrated loop ensures that models incorporate state-of-the-science knowledge about critical systems and then guide field and laboratory research.

(4) the interactions among these first three areas, and (5) modeling watershed and terrestrial processes at soil pore to global scales. As in the Watershed Sciences and Coastal Systems domains, BER Terrestrial Ecology excels at integrating multiple disciplines. Research in this domain focuses on the carbon cycle (a historical strength for DOE), climate feedbacks, nutrient cycling, and plant community structure and function, and is poised for new advancements in these areas. At the same time, respondents noticed gaps in research underpinning climate change mitigation and land-atmosphere interactions. From an international perspective, the evaluation team noted a weakening of the U.S. position in classical soil science.

Large-Scale Ecosystem Experiments and Integrative Research

BER has invested in national laboratory development of novel experimental approaches, such as FACE and deep soil warming (e.g., SPRUCE), to determine ecosystem response to increased atmospheric CO_2 concentrations. These approaches serve as valuable resources for the academic community and as templates internationally.

ModEx

According to interviewees, ModEx represents a signature BER approach for conducting ESS research. The term "ModEx" was rolled out at a 2012 workshop sponsored by BER's Terrestrial Ecosystem Science program, which was recently folded into ESS. BER has since become widely recognized for investing in this approach and implementing it across ESS domains. National and international communities view ModEx as a framework that enables rapid progress in new topical areas, helps effectively determine research priorities, and provides a powerful means of connecting domain knowledge with modeling (see Case Study: Next-Generation Ecosystem Experiments, p. 51).

Model Development and Use

U.S. and international science leaders recognize DOE leadership in land model development—including E3SM's Land Model (ELM) and the Functionally Assembled Terrestrial Ecosystem Simulator (FATES). Other noted achievements include process representations, close linkages to data and experiments, and the use of multiple teams or model tracks to develop alternative modeling approaches. One aspect of ModEx that received mixed reviews is the tasking of most terrestrial research (through guidance to SFAs, NGEEs, and university awards) with improved representation of terrestrial processes in land models that are fit for ESMs. Some respondents applauded this focus, but others noted that it can displace worthy priorities such as development of new theory and principles or high-risk, high-payoff discovery science. However, FOA awards for exploratory research have yielded positive outcomes for these other priorities (U.S. DOE 2020a; ess.science.energy.gov/summary-of-environmental-system-science-projects-awarded-in-summer-2021/).

4.2.4 Watershed Sciences

ESS watershed scientists are renowned for research that employs multiscale system science to integrate multiple disciplines in physical and natural sciences and often use a ModEx approach. ESS is particularly well-regarded for leadership in coupled hydrology and biogeochemistry, including using high-performance computing for reactive transport modeling of biogeochemical systems, exploring surface water–groundwater interactions, and linking microbial molecular biology to function and ecosystem impacts. ESS uses a community approach to tackle challenging watershed problems that have remained unaddressed. Examples include the Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds project and the Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems (WHONDRS).

Watershed Sciences SFAs funded by ESS have developed significant field infrastructure (coupled to numerical modeling systems) at multiple testbed sites across the continental United States. These testbeds provide community research sites and resources (see Fig. 4.5, p. 52). Several interviewees described the sites, especially the East River site in Colorado, as operating at unparalleled scales of collaboration for site-specific watershed research. These community testbeds are also a locus of some interagency collaboration.

Respondents also recognized BER watershed researchers for their leadership in integrating advanced technologies, such as artificial intelligence (AI), machine learning (ML), and cutting-edge analytical and computational capabilities. BER supports this strength with laboratory investment that emphasizes model enhancement and ModEx, while also supporting a broader range of use-inspired science for university-led and exploratory projects.

4.2.5 Coastal Systems

Although a nascent development within ESS, Coastal Systems represents a potential area in which BER can build its leadership. Researchers pursue holistic,

Continued on p. 52

CASE STUDY

Next-Generation Ecosystem Experiments

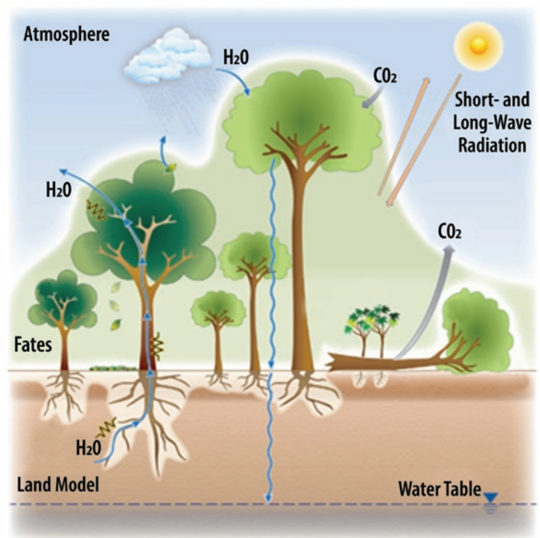
Thought leaders frequently referenced the positive paradigm shift achieved through Environmental System Science (ESS) program investments in Next-Generation Ecosystem Experiments (NGEE)—with one NGEE operating in the Arctic and another in the tropics. Each project has the goal of "advancing scientific understanding and model representation of poorly understood, climatically sensitive, and globally important ecosystems." This explicit connection to models, focusing on the DOE Energy Exascale Earth System Model (E3SM), benefits from core capabilities provided by DOE's national laboratory system, such as high-performance computing. NGEE projects also seek to build strategic partnerships between BER and universities, corporations, communities, and international organizations while facilitating close integration of empiricists and modelers.

The model-experiment (ModEx) framework lies at the heart of both NGEE projects, enabling rapid progress toward process representation in models, providing an effective way of determining research priorities, and creating strong connections between domain knowledge and modeling. For example, executing a ModEx framework in NGEE Tropics requires developing and testing model structures that represent tree functional diversity, heterogeneous availability and use of plant resources, and the ability to carry out fully coupled simulations in E3SM. E3SM's new hierarchical, modular modeling platform, called Functionally Assembled Terrestrial Ecosystem Simulator (FATES), integrates crucial processes of plant demography, ecophysiology, belowground biogeochemistry, and aquifer-to-canopy hydrology (see figure). FATES promises an improved understanding of how diversity in plant functional traits governs the responses of tropical forest ecosystems to climate and land use changes, and how that diversity ultimately determines tropical forest carbon, water, and energy feedbacks to the Earth system.

Although the NGEE projects are separately focused on model development and testing in tropical forests and Arctic tundra, both coordinate with model advancements taking place across other DOE-supported projects. These include AmeriFlux, Interoperable Design of Extreme-scale Application Software (IDEAS), fate and transport models such as the Parallel Reactive Flow and Transport (PFLOTRAN) model, the Atmospheric Radiation Measurement (ARM) user facility, model evaluation toolkits such as the International Land Model Benchmarking (ILAMB) project, and the ESS-sponsored Data Infrastructure for a Virtual Ecosystem (ESS-DIVE).

Takeaway

Explicitly connecting understanding of ecosystem processes to Earth system modeling is a paradigm shift in the integration of modeling, experimentation, and observations.



Next-Generation Dynamic Vegetation Model. The Functionally Assembled Terrestrial Ecosystem Simulator (FATES) is a dynamic vegetation model that predicts tree size distributions, disturbance dynamics, and plant trait competition. FATES has been integrated into the Energy Exascale Earth System Model and released as an open-source tool to the public. Because FATES makes predictions about tree size distributions, disturbance dynamics, and physiological dynamics at the level of individual trees, it can be more robustly tested against field measurements and can therefore serve as an organizing model for DOE field activities, particularly in forested ecosystems such as NGEE Tropics. [Courtesy Lawrence Berkeley National Laboratory]

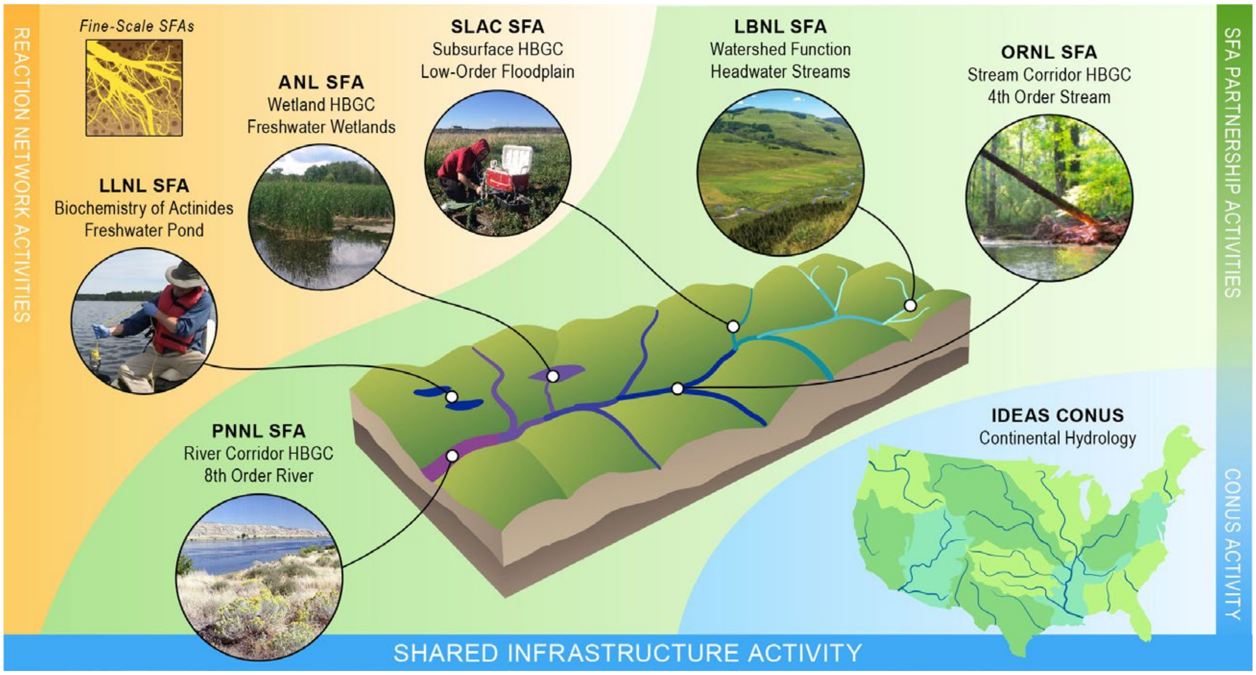


Fig. 4.5. A Community-Based Approach to Software Development. The Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds project seeks to enhance scientific productivity by adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem. Six major research activities, or Science Focus Areas (SFAs), address important scientific challenges, provide community research resources, and foster interagency collaboration. IDEAS-Watersheds aims to advance systems-level understanding of how watersheds function and to translate that understanding into advanced, science-based models of watershed systems.

Continued from p. 50

hypothesis-driven studies that integrate modeling and experiments to achieve system-level understanding of coastal processes and rivers and their representations in scale-aware, process-rich modeling frameworks.

Exemplifying the multidisciplinary science characteristic of ESS, Coastal Systems research combines the strengths of Watershed Sciences and Terrestrial Ecology to address new challenges specific to coastal regions. These challenges include nutrient cycling and fluxes in and across coastal zones and their impacts on global climate, coastal-urban interactions, impacts of sea level rise and other hydrological changes on erosion and human infrastructure, and vulnerability of coastal systems to climate change and other disturbances.

Much of the intellectual effort in the Coastal Systems domain targets interfaces and transition zones between terrestrial and aquatic environments because of their great complexity, considerable uncertainty about their response to environmental change, and potentially outsized impact on local-to-global Earth system processes. These efforts integrate prior ESS expertise in watershed and terrestrial systems. Respondents identified several opportunities to build upon this knowledge and expand leadership in Coastal Systems science, including human-natural system interactions and urban effects, given population concentration along coastlines. They encouraged continued development and application of ESS's unique research attributes to the emerging Coastal Systems area, including the ModEx approach, strengths in multidisciplinary system science, hydro-biogeochemical expertise, and strong mechanistic modeling capabilities.

Coastal Systems science has the potential to become a valuable integrator across disciplines, domains, and coupled systems, and DOE investment will infuse additional disciplines into this research area. However, the new coastal effort would benefit from better articulation of BER interests and integration with university and other domain experts. Because BER investment in coastal research is relatively new, the program needs to engage and recruit scientists from outside the national laboratory system to build the expertise needed to leverage existing progress on methods and major science questions rather than reinventing the wheel. This approach would be analogous to development of the NGEE Arctic and NGEE Tropics projects, which required time to establish national laboratory expertise, partnerships, and FOA capabilities. Unlike the NGEE start-ups, however, respondents noted that funding for the Coastal Observations, Mechanisms, and Predictions Across Systems and Scales (COMPASS) project and other major coastal investments is concentrated in fewer institutions, potentially limiting valuable two-way interactions with the university community.

4.2.6 ESS-Supporting Facilities and Infrastructure

BER supports national and international ESS research through its three scientific user facilities and sustained investments in experimental and data infrastructure for ecosystem studies. ESS research also is supported by additional DOE Office of Science facilities and resources including supercomputers, particle accelerators, X-ray light sources, and nanoscale science research centers.

BER's three user facilities serve ESS researchers around the world in large numbers, demonstrating their value as distinctive and global scientific resources (see Ch. 6: Enabling Infrastructure, Fig. 6.1, p. 85). These facilities are: (1) the Atmospheric Radiation Measurement (ARM) user facility; (2) Environmental Molecular Sciences Laboratory (EMSL); and (3) Joint Genome Institute (JGI). While known for their unique and sophisticated instrumentation, these user facilities provide equally important expert support in data interpretation, processing, and curation.

JGI provides BER with foundational strengths in understanding environmental microbiomes and microbial function. EMSL contributes to BER excellence in terrestrial and aquatic biogeochemistry and helps link information on genomics to ecosystem function. Respondents note that access to these facilities could be improved by providing potential users with (1) information on how to meet and work with facility staff and (2) facility assistance and guidance during the development of proposals to increase chances of success. Problems arise when proposals are expected to demonstrate access to needed facilities, yet those same facilities require DOE funding before confirming access.

ARM and AmeriFlux are additional examples of BER's long-term investments in data and observational infrastructure. ARM provides data for research on land-atmosphere interactions and validation of E3SM land models. The AmeriFlux Network, served by the AmeriFlux Management Project, is a collection of long-term, eddy-covariance flux stations that measure ecosystem carbon, water, and energy fluxes across the Americas. Respondents noted AmeriFlux's success in data accessibility and usage. Productive synergies between ARM and AmeriFlux demonstrate cross-program BER activities, including shared Small Business Innovation Research topics, workshop co-sponsorships, and AmeriFlux contributions to ARM campaigns. However, a gap exists between BER programs studying land fluxes versus atmospheric dynamics. Efforts to bridge this gap could entail, for example, funding from BER's Atmospheric System Research program for work outside of ARM measurement zones (which could, for example, extend NGEE studies to the atmosphere and climate) or for broadening these zones to include augmented terrestrial flux sites.

In addition to its user facilities, BER is known for large, sustained investments in (1) ecosystem experiment infrastructure such as SPRUCE and FACE; (2) community science sites, including the East River Watershed Function SFA study site; and (3) measurement and data infrastructure such as the AmeriFlux Management Project and Environmental System Science–Data Infrastructure for a Virtual Ecosystem (ESS-DIVE).

Respondents highlighted the critical contributions of many of these resources to U.S. scientific standing and success and to BER leadership in its topical domains. Moreover, this infrastructure demonstrates how BER investment in national laboratories positively impacts university scientists.

Historically, large-scale ecosystem manipulation experiments have been hallmarks of BER international leadership. The program has pioneered new designs adopted by research teams around the world, and many different projects are served by ongoing BER-supported experiments. However, BER has launched few large-scale manipulation experiments since the FACE program in 1980 and SPRUCE in 2010. International leadership in this area is shifting to Europe and Australia, which fund national and international manipulation experiments aimed at reducing uncertainty about ecosystem response to global climate change.

Large-scale manipulation experiments offer unprecedented opportunities for cross-disciplinary research that can bring together different ESS domains focused on understanding whole-ecosystem responses to drivers of climate change. A key challenge for BER will be to understand how investments in manipulation experiments, and perhaps coordinated observational networks, can best advance mechanistic understanding of ecosystem responses to climate change and how that understanding can be scaled to reduce uncertainty in climate change projections and resulting impacts on natural and managed ecosystems.

4.2.7 Data Access and Repositories

Respondents positively viewed DOE's new data management and data sharing policy, which brings ESS in line with best practices. In addition, BER culture is shifting in favor of submitting data to repositories and openly sharing data. For example, ESS has invested in ESS-DIVE as a framework for long-term data storage, sharing, and access and also in the development of community-based data and metadata standards. EMSL has invested heavily in its Network for Execution of User Science, or NEXUS (nexus.emsl.pnnl.gov/Portal), an integrated system for managing and accessing scientific data and for interfacing with users for proposal and project management. These activities and crowdsourcing efforts such as WHONDRS and COntinuous SOil REspiration (COSORE), a community database for continuous soil respiration and greenhouse gas flux data, provide opportunities to expand ESS into new territories.

Nevertheless, the discoverability of ESS data lags some other scientific fields. One challenge is that most ESS projects generate small or unique datasets that require detailed metadata for discovery and interpretation. Additionally, the large variety of data types complicates efforts to establish reporting standards, thus necessitating alternative innovative methods for data discoverability. These challenges are common to international research in environmental system science and require large investments to overcome. One international respondent identified data archives and data management as a major weakness of the United States, and particularly DOE, noting that some European countries invest much more funding. For example, Germany currently invests $85 million per year in developing and maintaining environmental data repositories and training scientists to use them. BER is not yet well-recognized for investments in data services in the United States, having invested in data infrastructure much later than, for example, the Consortium of Universities for the Advancement of Hydrologic Science, Inc. Even though significant BER investments exist (e.g., ESS-DIVE, EMSL NEXUS, National Microbiome Data Collaborative, JGI data, Earth System Grid Federation, ARM, and AmeriFlux), few are currently recognized internationally or even domestically outside of BER, thus further hampering the discoverability of rich ESS data holdings.

4.3 Future Opportunities

4.3.1 Integrate Human-Natural Systems into ESS

A concern mentioned frequently by respondents is ESS's lag in addressing fundamental science questions related to coupled human-natural systems relative to national and international peer programs. BER science is viewed as not adequately acknowledging the importance of managed landscapes, urban systems, coasts, estuaries, and regional extremes. One senior researcher stated, “the Office of Science has narrowly defined its science scope, ignoring the fundamental work needed to better understand coupled human-natural systems.”

BER projects like the Watershed Function SFA, NGEE Arctic, and NGEE Tropics represent internationally leading research investments that leverage sustained novel observational campaigns to achieve breakthroughs in advanced modeling of Earth system processes. A respondent noted, “BER could expand upon this strength to include more fine-scaled human systems and built-environment processes of relevance to energy and water resilience in the face of environmental stress.”

BER has taken a step in this direction with its recent funding opportunity announcement (U.S. DOE 2022b) for Urban Integrated Field Laboratories (IFLs). Investment in this unique and potentially world-leading endeavor builds on previous BER progress in integrated science to inform complex multisectoral interactions among human and environmental systems in urban contexts. Such synergies are also relevant to coastal systems, the AI for Earth System Predictability (AI4ESP) workshops, and the growing focus on mountainous hydroclimatic systems. Another respondent noted as an example, “if the E3SM modeling program sought to build a global climate model optimized for understanding regional-scale environmental extremes in human-influenced geographic contexts, this would lead to different scientific questions, model development focal areas, observational requirements, experimental methods, and so on. This is a space that BER is poised to lead in a big way if it chooses to do so but is currently only addressing in a handful of projects rather than treating this as a larger programmatic priority.”

The congressionally approved formation of urban IFLs represents a unique, immediate opportunity to couple human-natural systems research, with the goal of advancing understanding of these integrated systems in an urban context and providing the scientific underpinnings to equitably increase resilience to climate extremes (Geernaert 2021). ESS will lead the first urban IFLs, setting the stage for this program to identify the environmental system science grand challenge and use-inspired questions related to coupled urban systems. BERAC encourages ESS to generate these questions and related objectives by seeking input from university, national laboratory, community, and federal stakeholders.

Respondents and working group members concurred that BER should maintain its support of fundamental basic research as it pursues a focus on human-natural systems. Because environmental systems are impacted by human influence—even in landscapes that at first appear to be undisturbed—human-natural systems can be studied outside of managed landscapes (e.g., urban environments and agriculture). The effects of humans on natural systems include legacies from mining and timber harvest, changes to atmospheric composition (e.g., CO_2), and shifts in hydrological and major biogeochemical cycles due to climate change. In many cases, new discoveries could be achieved simply by recognizing the anthropogenic footprint in basic-research projects.

4.3.2 Develop Data as a Resource

Innovation is needed in managing and analyzing the increasingly large data volumes produced and required by advanced conceptual, modeling, and analytical capabilities in ESS. The program has the opportunity, and perhaps responsibility, as a producer and steward of large data holdings to expand strategies, procedures, and technologies for generating inferences from gigabyte- and terabyte-sized experimental datasets. Examples of large datasets from ESS studies include output data from an advanced mass spectrometer or data for a 3D tomographic analysis of a single sample.

Potential solutions for learning from large datasets include development of:

- Interpretative software tailored to specific methods, such as mass spectrometry or tomography.
- Strategies for data organization and database structures.
- Frameworks that facilitate data access and sharing in the context of intellectual property management.
- Secure yet highly accessible long-term storage.

BER has supported significant advancements in data management and analysis including EMSL's development of CoreMS, a comprehensive mass spectrometry framework for software development and data analysis of small molecules; FREDA, the FT-MS R Exploratory Data Analysis tool (shinyproxy.emsl.pnnl.gov/app/Freda) for analysis and visualization of Fourier transform mass spectrometry data; and the data management systems described in Section 4.2.7 (see p. 54). Respondents noted opportunities for ESS to enhance these activities to ensure that large data volumes generated by program research are ultimately translated into new theoretical developments. Capitalizing on these opportunities will enable ESS to assume leadership in a critical science area that involves all BER objectives.

A growing international emphasis on "Big Data," AI, and ML offers a promising opportunity for the scientific community to gain new insights from ESS data. However, endeavors that leverage these capabilities must be carefully managed and well described and communicated to avoid introducing fluctuations in research priorities. Respondents commented favorably on the partnerships developed through DOE's Advanced Scientific Computing Research program and its Scientific Discovery Through Advanced Computing (SciDAC) effort, which complement ESS interests. Taken together, these resources position BER to lead new data science initiatives, such as model integration with very large datasets (e.g., ModEx 2.0), hybrid approaches of data-driven and theory-driven models, and new theoretical approaches to causality.

4.3.3 Increase Crosscutting Activities

ESS leads in cross-scale science, but several themes remain siloed. Respondents noted the presence of obvious complementary capabilities across the research portfolios of BER's Earth and Environmental Systems Sciences Division (EESSD) and its Biological Systems Science Division (BSSD), yet co-funding or other explicit support for cross-division activities is often lacking. Environmental genomics is an example where cooperation or coordination between divisions might yield fruitful outcomes.

A key avenue for linking ESS and BSSD research would be efforts to develop a mechanistic understanding of how organisms (i.e., at the organismal level) drive ecosystem responses. However, a National Academy of Sciences member assessed BER as "currently lagging in ecophysiology." Similarly, a recipient of the Presidential Early Career Award for Scientists and Engineers assessed BER as having missed opportunities in linking organismal physiology to ESMs and to molecular biology, stating that "understanding basic mechanisms that underlie ecosystem responses is key." Furthermore, while AI and ML hold great promise, they cannot be relied upon alone for advancing mechanistic insights essential to understanding and projecting ecosystem responses to the "no analog" or "out-of-sample" environmental conditions facing future ecosystems. One respondent noted the need for creative approaches and deliberate initiatives that integrate mechanistic and scale information in pursuit of scaling laws that enable investigation of chemical, physical, and biological phenomena across scales.

Several experts noted the value of ESS leadership in open community science and encouraged a continuing focus and expansion of activities. The ESS workshop titled "Open Watersheds by Design" (U.S. DOE 2019) provided a framework for community-based science that continues to influence many BER, and specifically ESS, program elements. Respondents noted many examples of BER leadership, including (1) data collaboratives like AmeriFlux's partnership with FLUXNET networks, the National Microbiome Data Collaborative, and ESS-DIVE; (2) crowdsourced data collection, analysis, and publication efforts such as the WHONDRS international early career observational network-of-networks; and (3) collaborative modeling activities supported by DOE and other agencies and institutions (see Case Study: IDEAS—Interoperable Design of Extreme-scale Application Software, p. 57).

4.3.4 Prioritize Discoveries and Applications

ESS research findings could underpin solutions to multiple environmental problems such as water quality, ecosystem restoration, soil carbon storage, fire management, and coastal resilience. Thus, this report

Continued on p. 58

CASE STUDY

IDEAS—Interoperable Design of Extreme-scale Application Software

A family of projects called Interoperable Design of Extreme-scale Application Software (IDEAS) aims to increase scientific productivity in DOE Office of Science programs by accelerating software development and improving software sustainability in high-performance computing applications (ideas-productivity.org). IDEAS is creating a scientific software ecosystem comprising reusable, extensible, and interoperable software components and libraries. It also promotes best practices through education and outreach.

The Environmental System Science (ESS) program currently funds the IDEAS-Watersheds project, a collaboration among all six ESS-supported watershed Science Focus Area (SFA) projects. Jointly, the SFA teams are building an ecosystem of community codes in which modular components of various codes can be linked interoperably to efficiently develop models with needed functionality for a particular simulation problem (see figure).

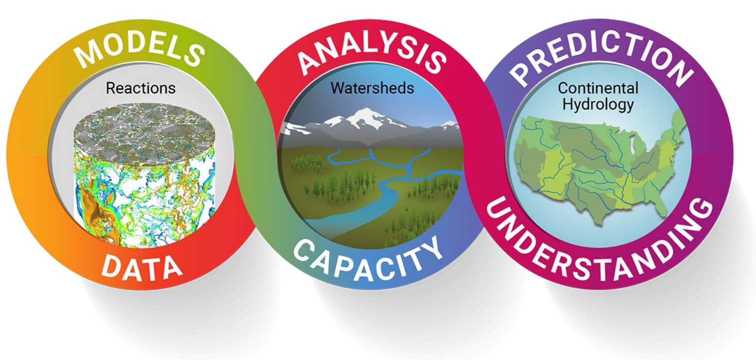
IDEAS exemplifies the community collaboration approach encouraged by ESS. The interoperable design enables individual labs, projects, and investigators to creatively develop their own codes, as opposed to a single code imposed on all, while optimizing productivity and sharing of high-quality code modules. For example, the Alquimia interface allows users of any hydrodynamics code to utilize well-established biogeochemistry modules within the PFLOTRAN or CrunchFlow models without intrusive code modifications or capability duplications.

Takeaway

A community approach has enabled leadership in the computational modeling of terrestrial and watershed ecosystems with high process fidelity at various spatial scales.

IDEAS-Watersheds is also building linkages between watershed and terrestrial models as well as microbial modeling tools in the DOE Systems Biology Knowledgebase (KBase) platform (kbase.us/multiscale-microbial-dynamics-modeling), thereby encouraging new cross-division collaborations within BER. This community approach has enabled ESS researchers to develop leadership in computational modeling of terrestrial and watershed systems with high process fidelity at a variety of spatial scales.

ESS codes are widely used around the world, including at DOE-funded leadership-class computing facilities, and in many cases are recognized as the gold standard of high-fidelity simulation tools. The ESS computational ecosystem fills a unique niche in high-fidelity process simulation of complex environmental systems, but this specialization may limit broad application outside DOE because the technology requires a high level of domain and computational expertise as well as access to high-performance computing hardware resources.



Software Ecosystem Improves Scientific Productivity. The Interoperable Design of Extreme-scale Application Software (IDEAS)–Watersheds project advances an ecosystem of interacting software tools and workflows that can be shared across all ESS-supported watershed Science Focus Areas. IDEAS facilitates the scaling of process understanding and simulation across scales. [Courtesy Los Alamos National Laboratory]

Continued from p. 56

recommends efforts to facilitate translation of ESS research to applications, solutions, and innovation by connecting information across all levels of research and development.

Placing a priority on both discovery and applications may seem contradictory, but experts contend that science is a pipeline—from grand challenge research to use-inspired discovery to applied science and finally to development and deployment—and the pipeline operates best when the components are connected. Awareness of advancements and gaps in one pipeline component can stimulate advancements in another. Conversely, isolating components can increase lag times between discovery and applied solutions or result in duplication of efforts.

4.3.5 Explore Additional Frontiers

Respondents identified additional scientific frontiers where BER's leadership could benefit the scientific community:

- **Disturbance and Extreme Weather Events**. BER leadership in this area would support DOE missions in climate, resilience, and water resources. Disturbances and extreme weather events, such as wildfires and flooding, and recurring non-steady-state systems, such as variable hydrological environments (e.g., tidal, tidal flats, streams, estuaries, and variable inundation wetlands), comprise a broad topical area that would build on and leverage BER strengths in modeling, data-model integration, multidisciplinary science, and MultiSector Dynamics.
- **Land-Atmosphere Interactions**. ESS could uniquely contribute to research on land-atmosphere interactions, namely the forces controlling water, energy, and chemical transfers between ecosystems and the atmosphere, which strongly influence convection, precipitation, and extreme events over land. Exciting potential exists to extend ESS's "bedrock-to-canopy" vision to include the atmosphere through hallmark BER programs like the NGEEs, SFAs, and AmeriFlux modalities. EESSD's Atmospheric System Research program and ARM user facility have expertise and mobile facilities that could enhance collaborations with the ESS program.
- **Real-Time Observations of Process Dynamics.** Using a next-generation light source or implementing new ways to distribute sensors in the field would advance real-time observations. The ability to connect and control sensors in the field and laboratory and then link them to simulation models could potentially revolutionize the integration of modeling and observations to guide experiments in real time. BER development of digital and real-life twin ecosystem approaches exemplifies this capability.
- **Scaling Laws for Coupled Hydro-Biogeochemical and Other Processes.** ESS should consider developing scaling laws for critical processes at different spatial scales simultaneously. This thrust would capitalize on BER strengths in multiscale science (e.g., from nanometer to catchment to climate scales), in specialized observing and analytical facilities, in modeling capabilities extending from molecules to genes to ecosystems, and in the AI and ML approaches outlined in Section 4.3.2 (see p. 55).

4.3.6 Maintain Strengths

BER has a strong reputation as a global leader in environmental system science. To maintain and strengthen this position, BER must preserve its strategic programmatic strengths in supporting cutting-edge environmental system science research that addresses consequential topics. Maintaining these strengths may include continuing to focus on the topics and processes underlying current successes but will also require adopting new perspectives on environmental research, including the role of human impacts. BER must evolve its scientific ideas and directions to fulfill DOE's mission in a changing world and to maintain ESS's international status. One respondent summarized this with the statement that "mission-oriented discovery research is the correct formula for long-term relevance and impact."

4.3.7 Additional Recommendations

Feedback from respondents included praise for BER's strengths and encouragement to continue building upon identified opportunities. Some of the comments and recommendations are highlighted below:

- Communicate BER strengths more effectively, including the program's world-class projects; unique facilities; and leadership in creating synergies across observations, process studies, and systems modeling capabilities.
- Pursue or articulate a refined focus for certain initiatives (e.g., coastal ecosystems, Arctic, tropics) to distinguish them from the many other research programs in this space.
- Integrate microbiomes, multiomics (JGI), analytical capabilities (EMSL), atmospheric measurements (ARM), and data analytics expertise more deliberately within ESS research.
- Accelerate discovery and design applications for DOE-relevant human-security questions by taking advantage of BER expertise in AI, ML, and quantum computing for the Global Change Intersectoral Modeling System (GCIMS), E3SM, and Integrated Multisector Multiscale Modeling (IM_3) programs.
- Place more emphasis on uncertainty quantification and uncertainty propagation through complex, multiscale systems in modeling activities.

4.4 Outlook for BER Leadership in Environmental Sciences

4.4.1 Respondent Suggestions

With its current approach, ESS has successfully implemented a broad portfolio of environmental science research themes and funding modalities. Continuing to pursue success with the same efforts may be tempting, but most respondents proposed specific ideas or posed questions about the trajectories of current activities that could impact the future of ESS research. This feedback falls into five categories: (1) the research model for large, long-term projects (e.g., SFAs and NGEEs); (2) international collaboration; (3) ModEx; (4) model intercomparison projects; and (5) the promotion of a diverse, safe, and well-supported scientific workforce.

Large, Long-Term Project Model

Much of the positive international reputation of ESS science is attributable to the long-term nature and broad interdisciplinary team approach of the NGEE and SFA projects. Respondents did not identify any areas of concern regarding these projects' evolution. However, questions arose about the utility of such intensive place-based research, specifically in the context of portability. Some wondered whether the findings from these locations would be broadly applicable, a challenge common to all long-term research findings. Current approaches will likely continue to produce valuable discoveries. However, more impactful societal effects could be achieved by advancing studies that include humans in environmental systems. Building on the strengths of the NGEEs and SFAs, new long-term interdisciplinary projects might be designed to address identified ESS science challenges (i.e., human-natural system interactions) and consider new directions, such as the effects of climate change and disturbances (e.g., fires) on carbon cycling and feedbacks to broader systems. For example, ESS could support an NGEE- or SFA-equivalent project focused on managed lands, which would take advantage of BER strengths (e.g., biogeochemical reactive transport modeling) as well as expertise within other DOE programs, including Basic Energy Sciences (BES), and federal agencies such as USDA.

International Collaboration

ESS supports few international collaborations, yet its scientific priorities are not confined to U.S. borders. Globally significant initiatives, such as the study of soil carbon sequestration, are underway but operate under scientific uncertainties. Many discussions related to these initiatives happen among lawmakers and within the agricultural science community but could benefit from the deep fundamental understanding of environmental science available at national laboratories. For instance, applying basaltic rock as part of enhanced weathering strategies to sequester carbon in croplands requires careful evaluation using reactive transport modeling. This capability is available at national laboratories but not typically to communities seeking to benefit from carbon credits. Effectively addressing the multidimensional environmental science challenges in managed lands requires collaborations—both across DOE (e.g., BES and BER biogeochemical reactive transport modeling) and with international science groups and other federal agency scientists.

ModEx

The ModEx framework has contributed significantly to ESS success, achieving breakthroughs that otherwise would have taken much longer without the iterative cycle of refining and testing models with field and laboratory data, which is fundamental to the ModEx approach. However, despite overwhelming support for ModEx, respondents suggest that its evolution toward achieving scientific outcomes beyond model refinement must have either a conclusion or an evolution. One benefit of continuing to work within the current ModEx paradigm is the likelihood of greater model accuracy. A future in which ModEx evolves toward specific goals beyond model refinement may be one that more quickly identifies and supports fundamental and impactful discovery.

Many respondents described ModEx as a centerpiece of ESS research, bringing together different programs across EESSD. However, integration of multiscale models into programmatic research priorities can introduce perceived barriers if scientists do not have modeling expertise or interests. Empiricists, therefore, may question how best to engage with ESS given their career objectives and the mission-driven needs of the program. Respondents noted that clear communication could lower this barrier by easing or better describing the requirements of model-data integration within the Earth, environmental, and climate sciences.

Model Intercomparison Projects

Similar to ModEx, respondents questioned whether the model intercomparison projects (MIPs) will evolve to generate advanced science outcomes. As conceived, this framework has valuably contributed to model advancement and refinement, but ample opportunity exists for defining new ways of conducting MIPs with the goal of scientific discovery. A future direction that considers new purposes of MIPs versus their current usage could rapidly advance environmental science in new ways.

Diverse, Safe, and Well-Supported Scientific Workforce

Many respondents commented on issues related to workforce diversity, equity, and professional development and training (see Ch. 8: Strategies for People, Partnerships, and Productivity, p. 122, for an overarching and in-depth discussion of workforce issues). For ESS specifically, respondents noted that the program's current scientific workforce does not reflect the broad diversity of U.S. society and that postdoctoral and early career scientists lack training opportunities in proposal writing and project management.

Moreover, for some students, accessibility issues sometimes pose greater barriers to embarking on an environmental science career than academic training. For example, many students and early career scientists from urban areas, especially economically disadvantaged areas, lack the opportunity to engage in outdoor pursuits growing up and thus may be uncomfortable with conducting fieldwork. This inequity emerges long before opportunities arise to engage in DOE science activities. Within DOE, ESS is particularly well-positioned to see these impacts. However, ESS funds projects with excellent field research training and safety practices (e.g., NGEE Arctic) that could directly support a broader new effort to engage students who want or need to conduct fieldwork but have no experience.

BERAC encourages ESS to embrace opportunities to diversify its research community and to increase equity in field science by prioritizing field training and safety—changes that could become new hallmarks for ESS. Furthermore, a broader culture of safety, harassment prevention, and trust would greatly benefit all ESS science. Fundamentally, harassment in the field, or at any work location, is a safety issue, and thus ESS should institutionalize a new approach to field training and safety.

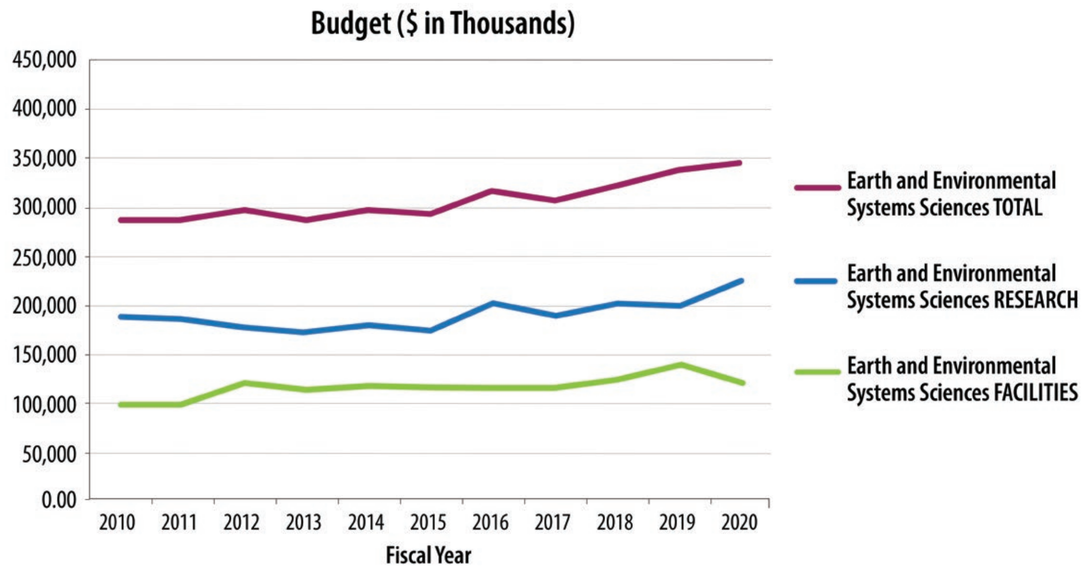


Fig. 4.6. BER's Earth and Environmental Systems Sciences Division (EESSD) Budget Trends Across 10 Years. [Courtesy DOE Office of Scientific and Technical Information]

4.4.2 Volatility and Uncertainty in Funding and Research Priorities

Budget uncertainties and rapid shifts in the focus of funded tasks are challenges that can inhibit ESS leadership potential. For example, international expenditures for environmental system science are growing while U.S. funding remains flat, and the ESS research community sometimes is not well prepared or positioned for fluctuations in program emphasis areas.

Appropriation and Allocation of Research Funds

Over the past decade, Congress has increased the funds appropriated to BER, which uses those funds to support research and user facilities. Overall, EESSD (and ESS) has seen similar increases during this time, though its funding has fluctuated year to year by –4.16% in FY 2013 to +11.78% in FY 2020 (see Fig. 4.6, this page). Although annual reductions in funding were small, respondents note that budgetary shortfalls disproportionally affect new research programs, university solicitations, and Small Business Innovation Research opportunities due to a need to maintain funding commitments on existing projects.

Also problematic are the evident tradeoffs between funding allocations to research programs versus user facilities (e.g., ARM and EMSL), but respondents broadly supported these complementary investments within EESSD and ESS. Indeed, the world-class staffing and capabilities of many user facilities are difficult or impossible to duplicate at universities and private companies.

When assessed in an international context, flat funding levels threaten BER and U.S. science leadership. European and Asian expenditures on ESS-relevant research and development (e.g., sustainability, environmental quality, and climate change) are meeting or exceeding U.S. funding, in terms of both spending as a percentage of gross domestic product and expanding their scientific workforces (see Fig. 1.3 and Fig. 1.4, p. 9).

Fluctuations in Research Priorities and Topics

Respondents lauded ESS's consistent-to-increasing budgets over the past decade but noted the program's dramatic organizational change 2 years ago coupled with a shift in how funds were allocated to research priorities. BER combined traditional programs (Terrestrial Ecosystem Science and Subsurface Biogeochemical Research), moved funding modalities incrementally to large projects and SFAs, and shifted strategic research priorities from the fate and transport of contaminants to watershed biogeochemical and hydrological processes.

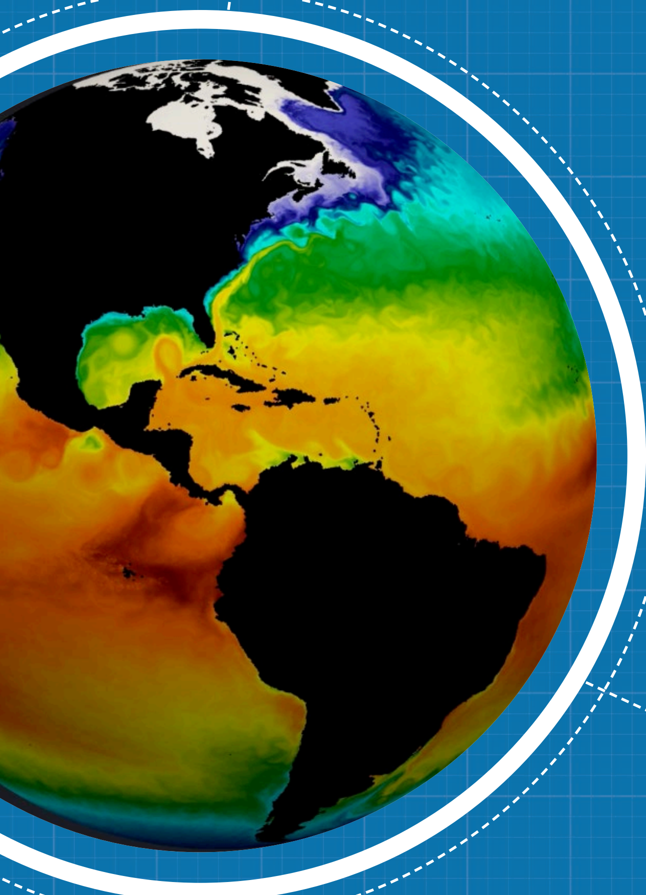
While this shift seemed abrupt at the time, BER effectively communicated the rationale for these changes in strategic plans, at annual principal investigator meetings, and via web content. However, several respondents were quick to add that ESS inclusion and funding of coastal projects were communicated less well. A 2017 workshop report on terrestrial-aquatic interfaces described some of the rationale for investing in coastal systems (U.S. DOE 2017), but the funding and evolution of such projects were not well communicated to the impacted ESS research community. Although ESS's new coastal research area can potentially expand and refresh the coastal scientific community, some respondents expressed concern that few scientists traditionally sponsored by ESS really understand these systems. Consequently, the ESS research community will have a steep learning curve requiring patience from both DOE and the broader community.

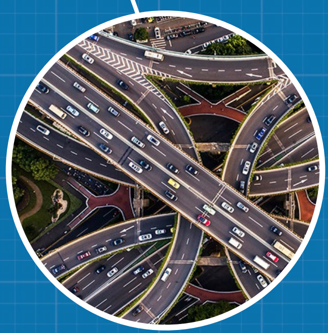
Respondents also emphasized the erosion of hallmark ESS capabilities in large-scale, long-term experiments (e.g., FACE) in recent years, suggesting the program guard this legacy and expand it.

Another program affected by organizational shifts is DOE's Early Career Research Program. In EESSD's implementation, a different program sponsors the Early Career awards each year. While potentially positive in theory, this approach results in dramatic changes to Early Career solicitation topics from year to year. Consequently, topics relevant to ESS researchers might only be available every 3 to 4 years and are not predictable from one cycle to the next. For many scientists, even anticipating the order of which program will sponsor a particular year's awards is not straightforward. This uncertainty introduces an element of being "in the right place at the right time," potentially limiting the award's intent to fairly recognize and support outstanding talent.

CHAPTER 5

Climate Science





Working Group Co-Leads

Shaocheng Xie, *Lawrence Livermore National Laboratory*
Ann M. Fridlind, *NASA Goddard Institute for Space Studies*

Working Group Members

Klaus Keller, *Dartmouth College*
Gerald A. Meehl, *National Center for Atmospheric Research*
Johannes Quaas, *Leipzig University*

Contributions of former BERAC member Dr. Katherine Calvin to this work prior to her full-time detail to NASA Headquarters are gratefully acknowledged.

Chapter 5
Key Findings and Recommendations

Key Findings

KF5.1 BER-funded climate science publications are among the most highly cited papers in the field, garnering a higher rate of citations than non-BER publications, particularly for the top 1% and 5% of papers.

KF5.2 BER has demonstrated international leadership in developing and interpreting climate model intercomparisons through the DOE Program for Climate Model Diagnosis and Intercomparison (PCMDI) and was a leading contributor to research earning the 2007 Nobel Peace Prize awarded to the Intergovernmental Panel on Climate Change and former U.S. Vice President Al Gore.

KF5.3 BER is a world leader in climate change and cloud feedback research through its application of the "fingerprint" method to identify signatures of human influence on climate and its development of innovative techniques to quantify cloud feedbacks and pin down equilibrium climate sensitivity.

KF5.4 BER has advanced exascale computing to become one of the world's leading developers of kilometer-scale Earth system models, such as the convection-permitting Energy Exascale Earth System Model.

KF5.5 BER has successfully developed capabilities in crosscutting energy-related research and coupled human-Earth system models, such as the Global Change Analysis Model.

KF5.6 BER leads internationally in capturing ground-based and aerial atmospheric measurements through its Atmospheric Radiation Measurement (ARM) user facility and in advancing physical understanding of atmospheric systems through the associated Atmospheric System Research program.

Recommendations

R5.1 Increase investment in development of kilometer-scale Earth system modeling by advancing exascale computing, artificial intelligence and machine-learning approaches, and model-observation integration.

R5.2 Strengthen international leadership in modeling the coupled human-Earth system by providing more decision-relevant insights and better accounting for model uncertainties.

R5.3 Sustain international leadership in ground-based and aerial measurements and their use in advancing physical process understanding by strengthening collaborations with the satellite community, supporting integration of national and international field-observing systems, and potentially establishing synergistic leadership in laboratory chamber facilities.

R5.4 Strengthen international leadership in model intercomparison activities and in climate sensitivity research by increasing support for PCMDI, the Earth System Grid Federation, and process-oriented exercises that use ARM observations.

R5.5 Establish sustained and substantial funding for expanded collaboration between U.S. agencies and universities to improve research outcomes and integration of efforts to meet societal needs.

R5.6 Create additional means for supporting "blue sky" proposals from DOE scientists to stimulate innovation and workforce engagement.

5 Climate Science

5.1 Overview of BER Climate Science

5.1.1 Atmospheric and Modeling Programs

BER conducts climate science research activities under three programs: the Atmospheric Radiation Measurement (ARM) user facility, the Atmospheric System Research (ASR) program, and the Earth and Environmental Systems Modeling (EESM) program (see Fig. 5.1, this page).

ARM supports well-instrumented ground research sites in the world's most important climate regions and co-located intensive field campaigns at appropriately short physical and temporal scales (arm.gov/about/history). Over the past 30 years, ARM has provided a growing suite of continuous measurements of surface radiative flux quantities, atmospheric state, trace gases, atmospheric aerosols, clouds, and precipitation. Field campaigns are supported at fixed and mobile surface sites via ARM mobile and aerial facility deployments and funding for domestic and international participants.

ASR supports the use of ARM observations and ancillary activities to advance process-level understanding of the key interactions among aerosols, clouds, precipitation, radiation, dynamics, and thermodynamics, with the ultimate goal of reducing the uncertainty in global and regional climate simulations and projections (asr.science.energy.gov). ASR activities are tightly coupled to ARM observations to advance understanding of atmospheric processes using a hierarchy of modeling scales ranging from box models to Earth system models (ESMs).

EESM seeks to simulate and understand DOE-relevant predictability of the Earth system (climatemodeling.science.energy.gov) through three program areas: Earth System Model Development, Regional and Global Model Analysis, and MultiSector Dynamics.

Fig. 5.1. BER Engages in Crosscutting Climate Research. Efforts in atmospheric sciences research, environmental system science, Earth system modeling, and data management incorporate the activities shown in the figure and are supported by various user facilities. Such cross-disciplinary approaches result in, for example, the high-resolution Energy Exascale Earth System Model (E3SM), which can simulate changes in water vapor (tan) and sea surface temperatures (red to blue) as a hurricane moves across the Atlantic Ocean toward the U.S. East Coast. The resulting cold wake affects subsequent intensification of the next hurricane. [Modeling visualization courtesy Los Alamos National Laboratory.]

Within the Earth System Model Development program area, EESM funds development, use, and analysis of the Energy Exascale Earth System Model (E3SM). E3SM is a fully coupled ESM with low-resolution (~100 km), regionally refined (25 km to 100 km), and high-resolution (~3 km) versions (e3sm.org). E3SM's core simulation campaigns focus on answering science questions related to the water cycle, biogeochemistry, and the cryosphere. Through the Regional and Global Model Analysis program area, EESM supports studies diagnosing and analyzing (1) state-of-the-science coupled climate models and ESMs; (2) climate sensitivity and feedbacks from various processes; (3) attribution and detection of climate change and climate variability; and (4) impacts of extreme events, especially droughts, floods, and tropical cyclones. Finally, within the MultiSector Dynamics program area, EESM analyzes interactions between human and natural systems and funds development of the Global Change Analysis Model (globalchange.umd.edu/gcam).

5.1.2 Leadership Assessment

This chapter goes beyond standard metrics, such as publication and citation numbers, to assess BER's international leadership role in the following areas: international committees, Intergovernmental Panel on Climate Change (IPCC) assessment reports, workshop and conference organization, and cutting-edge research and observations.

One indicator of international leadership by BER climate scientists is their participation in committees and working groups of the World Climate Research Programme (WCRP), a premier international organization prioritizing and coordinating climate science research around the world. WCRP engages climate scientists as volunteer coordinators and facilitators of international climate research to develop, share, and apply the climate knowledge that contributes to societal well-being (wcrp-climate.org). BER-funded scientists have consistently demonstrated leadership in committees and working groups for several of WCRP's six core projects (wcrp-climate.org/learn-core-projects), including the Coupled Model Intercomparison Project (CMIP), the Cloud Feedback Model Intercomparison Project, and the Global Energy and Water Exchanges Project. BER scientists have also participated in WCRP Grand Challenges (wcrp-climate.org/component/content/category/26-grand-challenges) and Lighthouse Activities (wcrp-climate.org/lha-overview).

Participation in WCRP enables BER-supported scientists to lead climate research that defines and addresses questions too large or complex to be tackled by a single nation, agency, or scientific discipline. These scientists can influence the international climate science research agenda through international coordination and partnerships and exchange information with BER program managers about compelling WCRP-relevant science questions. These questions may then be reflected in BER-funded research to advance understanding of the multiscale dynamic interactions between natural and social systems affecting climate. BER-supported researchers are widely distributed throughout the WCRP structure, with notable concentrations in the BER climate science focus areas, and thus play key international leadership roles in climate science.

Another indicator of international leadership is participation in the IPCC assessment process as contributors, lead authors, or coordinating lead authors of reports that assess human knowledge of climate change and variability. BER-supported scientists have participated in the IPCC assessment process and all six assessment reports. As contributors, they ensure that the IPCC properly evaluates DOE-funded research results. IPCC reports also regularly cite BER-supported research.

Finally, BER climate scientists lead in organizing international conferences, including serving on organizing committees and leading sessions at major climate science meetings organized by both professional societies (e.g., the American Geophysical Union and the American Meteorological Society) and BER-funded projects (e.g., ARM, Global Change Analysis Model, and AmeriFlux).

5.2 Leadership Status

Publication metrics provide a general overview of how BER-funded climate science compares to the rest of the world. Although BER-funded climate science papers represent only 1.8% of all climate publications between 2010 and 2020, they are cited more often than other publications, accounting for 4.2% of the top 5% most cited publications and 5.4% of the top 1% (see Table 5.1, p. 67). BER climate publications also garner more citations than non-BER publications, with an average 8 citations per publication per year compared to 6.1 for domestic and 3.9 for nondomestic publications. See Appendix C: Approach to Metrics and Methodologies, p. 151, for more details on publication metrics.

Table 5.1 BER Proportion of Climate Science Publications

Year	BER % All Pubs	BER Top 1%	BER Top 5%	BER Top 10%	BER Top 20%
2010	1.36%	3.49%	2.10%	2.68%	1.86%
2011	1.61%	7.45%	3.97%	3.18%	2.87%
2012	1.62%	7.69%	4.43%	4.14%	3.46%
2013	2.07%	10.08%	7.65%	5.56%	4.19%
2014	2.08%	3.23%	3.88%	4.33%	3.38%
2015	2.03%	2.99%	4.03%	3.94%	3.87%
2016	2.19%	8.39%	5.59%	4.52%	3.81%
2017	1.75%	3.29%	4.50%	3.59%	2.81%
2018	1.99%	3.59%	4.47%	3.54%	3.53%
2019	1.67%	6.18%	3.05%	2.75%	2.56%
2020	1.59%	2.99%	2.59%	2.87%	2.72%
Avg.	1.81%	5.40%	4.21%	3.74%	3.19%

BER-funded publications are disproportionately represented among highly cited climate science publications. Comparison groups are BER versus all other domestic and nondomestic publications. Top document categories are based on percentile distribution of publications by citation volume. [Courtesy DOE Office of Scientific and Technical Information]

The next six subsections evaluate BER performance based on information gathered from interviews with throught leaders and responses to a Request For Information in the specific areas of climate science that BER funds: ARM and ASR, Earth system modeling, human-Earth system modeling, model intercomparisons, cloud feedback and climate analysis, and enabling capabilities.

5.2.1 ARM and ASR

Nearly all interviewed respondents view ARM as a world leader in ground-based and aerial climate measurements, particularly in supporting field campaigns that bring additional instruments to its fixed and mobile sites (see Fig. 5.2, p. 68). ARM leads ground-based programs around the world in terms of combined data record length and breadth of measurement suites at fixed and mobile sites, diversity of conditions and locations monitored in climate-relevant areas, and influence in studying the climate system. ARM is also world-leading in data management, provision, and exploration, setting the standard for other climate-observing facilities internationally. ARM's lengthy data record is a particular asset for complex multidimensional statistical and trend analysis.

Respondents describe ASR as world leading in understanding atmospheric processes through its use of ARM process-oriented observations. Specifically, ASR leads in boundary layer and troposphere processes, aerosol and cloud microphysical processes, and aerosol-cloud interactions.

Together, ARM and ASR lead in connecting user facility data to global and regional model developments by promoting a hierarchical framework of process modeling that includes the single-column model, cloud-resolving model, large-eddy simulation models, and the Cloud-Associated Parameterizations Testbed (pcmdi.llnl.gov/projects/capt). This framework develops and tests atmospheric physical parameterizations and bridges the scale gap between ARM data and models. ARM and ASR scientists have led or co-led a growing number of process model intercomparison studies conducted by international modeling

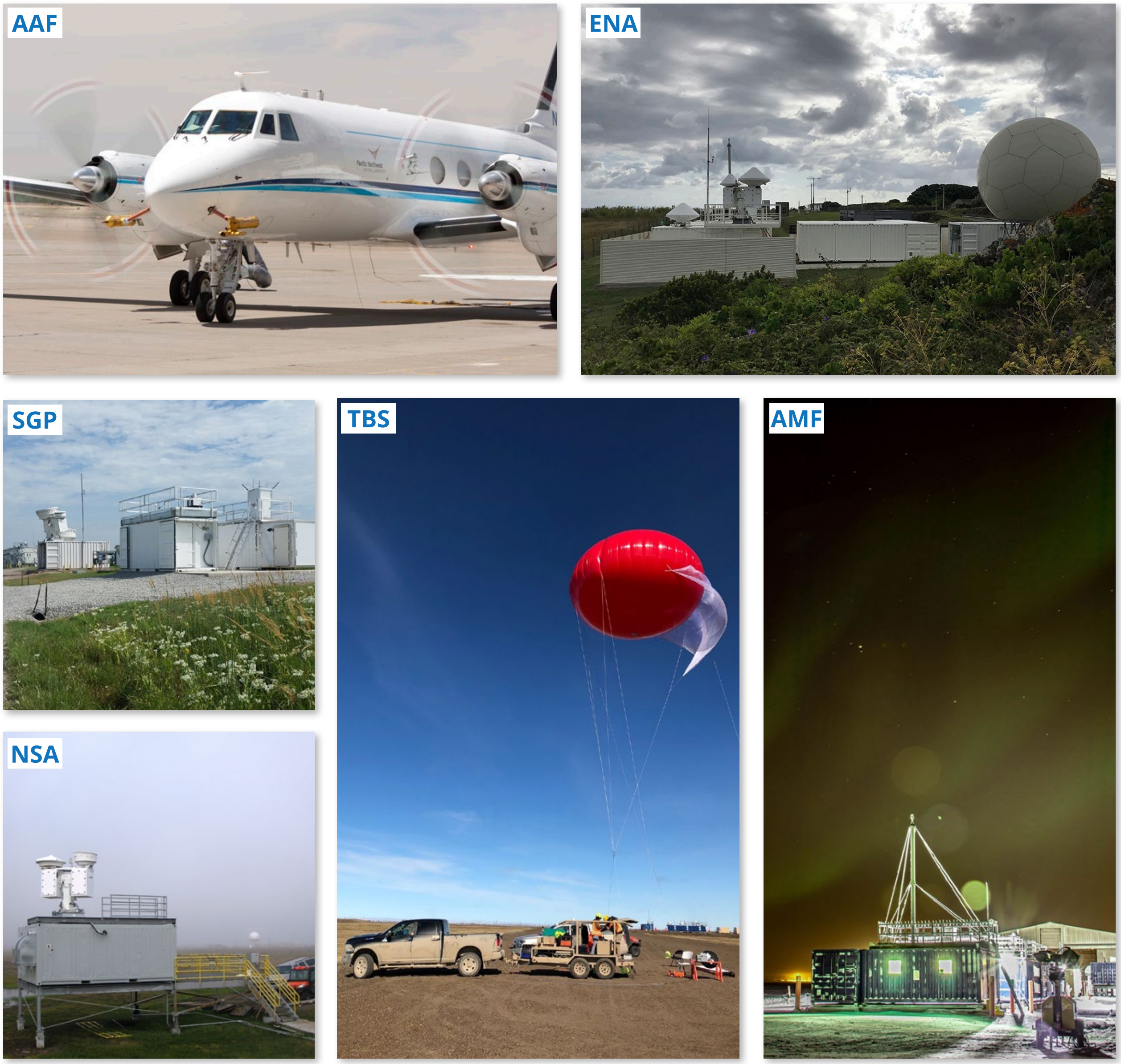


Fig. 5.2. BER Supports Worldwide Deployment of Atmospheric Monitoring Instrumentation. The Atmospheric Radiation Measurement (ARM) user facility provides comprehensive measurements for studying atmospheric processes in areas where they are most needed by the science community. Data are collected by the ARM Aerial Facility (AAF); ARM Mobile Facilities (AMF); tethered balloon systems (TBS); and three fixed atmospheric observatories in the Eastern North Atlantic (ENA), North Slope of Alaska (NSA), and Southern Great Plains (SGP). [All images courtesy ARM]

communities, including the Global Atmospheric System Studies Panel and the preceding Cloud System Study panel of the WCRP Global Energy and Water Exchanges Project. ARM's variational analysis forcing data (arm.gov/capabilities/vaps/varanal) has provided arguably the most widely used forcing data to support process modeling studies worldwide. The ARM Best Estimate data product (arm.gov/capabilities/vaps/armbe) has set a standard for creating climate model–friendly integrated data products for other observational programs or field campaigns such as the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) expedition (mosiaic-expedition.org).

Respondents noted a few areas that could be strengthened:

- While ARM excels at collecting climate and cloud measurements and BER programs support strong modeling efforts, ARM and ASR could increase involvement in laboratory studies as a third pillar of progress in the field. For example, DOE does not have any major aerosol and cloud chamber user facilities, which are now playing a leading role internationally in advancing understanding of aerosol and cloud microphysical processes. Accurately representing these processes is a major challenge of BER's climate model parameterizations.
- ARM field campaign data receive widespread use, but long-term data from ARM's fixed sites lack such a broad user community.
- Limited spatial coverage is another challenge for ARM, which may cause issues with physical parameterizations based on data collected at the limited number of ARM sites.
- Collaboration with the satellite community needs to be strengthened and could be achieved through stronger interagency partnerships at the national level under joint management (see Ch. 7: Integrative Science, p. 103).
- As the international community begins catching up to BER in some areas, such as well-calibrated long-term surface site network measurements, ARM should embrace the expanding community and seek to contribute new leadership roles, such as helping guide integration of U.S. and international climate-observing systems.
- ARM might benefit from leading or co-authoring a strategic plan to address the continuing interagency and international challenge of transferring knowledge from observations to global climate models in a more integrative way.

5.2.2 Earth System Modeling

With its recent development of E3SM, BER now leads convection-permitting climate modeling at the national level. E3SM is one of several Earth system models undergoing independent development in the United States today, along with publicly available models supported by the National Science Foundation (NSF), the National Oceanic and Atmospheric Administration (NOAA), and NASA. BER has demonstrated growing capabilities in Earth system modeling, with E3SM, and in coupling atmospheric, ocean, cryosphere, and land models. Some respondents were impressed with E3SM biogeochemistry modeling and viewed BER as a leader in regional and global model developments. Other respondents pointed to BER's E3SM performance in some areas as evidence that it will take time for the relatively new model to catch up with other world leaders in climate modeling such as NSF's National Center for Atmospheric Research (NCAR) and NOAA's Geophysical Fluid Dynamics Laboratory (GFDL). One respondent noted that the current E3SM lags in the area of chemistry, partly due to the high computational cost required to include complex atmospheric chemistry in the model. Another respondent perceived a major weakness in ocean circulation and ocean biogeochemistry in E3SM. Respondents also saw clear opportunities where BER could take a new leadership role, such as in biological aerosol modeling.

Respondents generally shared the concern that separating E3SM from the NCAR Community Earth System Model (CESM) might create unnecessary duplication of efforts and bifurcate the science community, even though E3SM enables BER to better address DOE's scientific objectives and connect its ESM development to other DOE-funded efforts. Areas needing growth include predictive skill, coupling of processes, and connection to DOE research in energy and human systems. One respondent suggested that DOE allocate resources toward efforts it already leads, such as computing and very high-resolution modeling, rather than using resources to catch E3SM up to groups with standard resolution versions (e.g., 1 degree down to ¼ degree).

Several respondents questioned why E3SM did not play a more prominent role in CMIP Phase 6

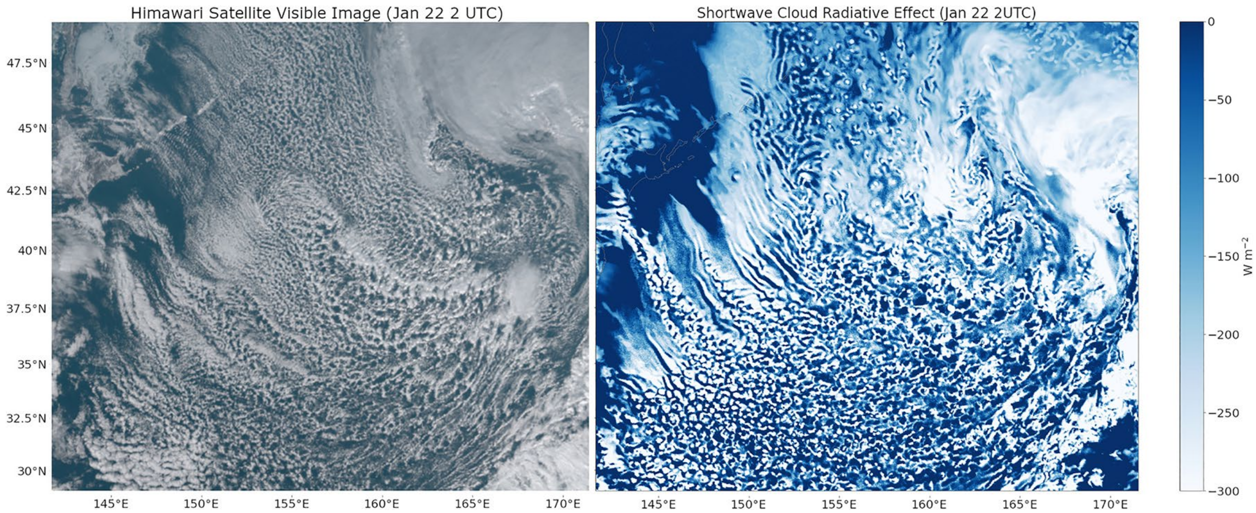


Fig. 5.3. BER Leads in Kilometer-Scale Physical Climate Modeling. Cold-air outbreak off Siberia on January 22, 2020, from a Himawari visible satellite image (left) and a snapshot of shortwave cloud radiative effect from the Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM; right). A comparison of the images reveals striking similarity between observed and simulated cloud structures, suggesting that SCREAM's combination of resolution and boundary layer and cloud parameterizations contains the physics necessary to capture cloud transitions in cold-air outbreaks. [Reprinted under a Creative Commons Attribution 4.0 International License (CC By 4.0) from Caldwell, P. M., et al. 2021. "Convection-Permitting Simulations with the E3SM Global Atmosphere Model," *Journal of Advances in Modeling Earth Systems* **13**(11), e2021MS002544.]

(CMIP6), potentially ceding international leadership, credibility, and prominence in Earth system modeling to other countries. However, another respondent supported the decision and urged E3SM scientists to focus instead on model development of kilometer-scale ESMs. One respondent also noted that the most ambitious kilometer-scale digital twin efforts in Europe will not participate in CMIP because their emphasis on data assimilation and shorter time frames is currently incompatible with CMIP.

Despite some mixed opinions, respondents agree that BER leads or has the potential to lead high-resolution climate modeling with its next generation of high-performance computing facilities. BER's current efforts to develop the global convection-permitting Simple Cloud-Resolving E3SM Atmosphere Model (SCREAM, e3sm.org/the-e3sm-nonhydrostatic-dynamical-core, see Fig. 5.3, this page) position DOE as an upcoming global leader in kilometer-scale physical climate modeling, with competition from only a few currently existing efforts [e.g., the Nonhydrostatic ICosahedral Atmospheric Model (NICAM) in Japan and the Icosahedral Nonhydrostatic Weather and Climate Model (ICON) in Germany]. Respondents commended BER's high-resolution modeling efforts and advocated continued pursuit, ideally in constructive collaboration with the wider U.S. climate modeling community.

An asset for DOE is that kilometer-scale modeling resolutions match kilometer-scale observations from satellite instruments, but the most internationally competitive high-resolution modeling may have moved toward digital twin efforts, which require data assimilation. Such work in Europe is accompanied by major investments to partner and exchange information with public and private stakeholders, as discussed further in Ch. 7: Integrative Science (see p. 103). One respondent noted a need to balance BER's high-resolution modeling efforts with its continuing improvements to the low-resolution E3SM; this would address BER's mission-driven questions related to coupled human-Earth system interactions and prognostic prediction of sea-level rise. For this work, E3SM requires a state-of-the-art, low-resolution model with major biases fixed because very

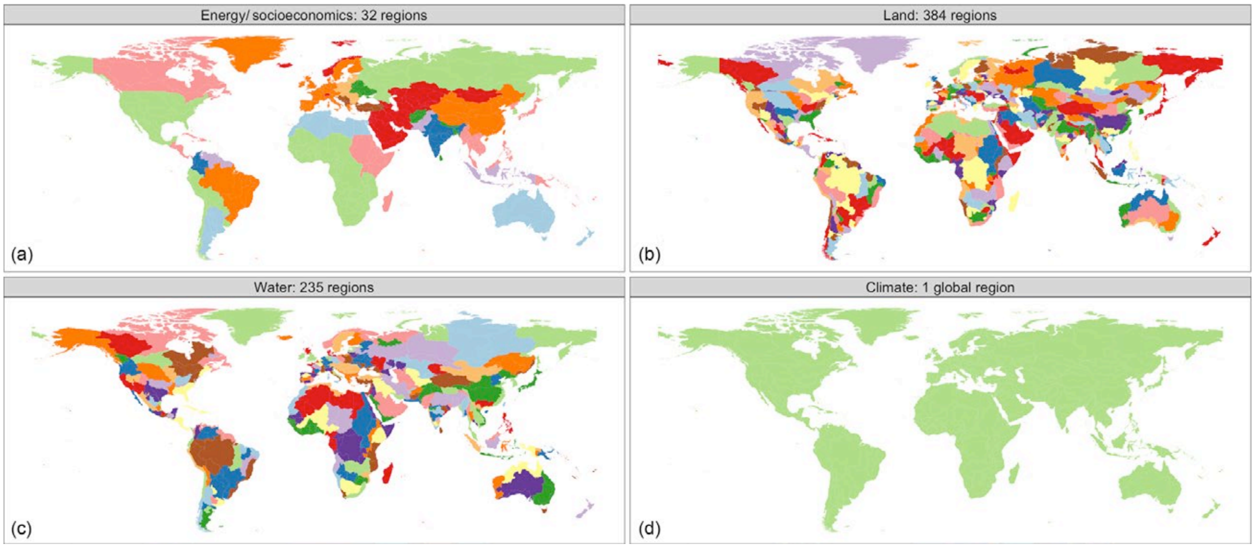


Fig. 5.4. Modeling Coupled Human-Earth Systems. The Global Change Analysis Model (GCAM) represents five different interacting and interconnected systems: energy, socioeconomics, land, water, and climate. The economic and energy systems are represented by 32 geopolitical regions **(a)**, providing insights about broad international socioeconomic and energy dynamics. The land system is based on a combination of geopolitical boundaries and water basins, resulting in 384 regions **(b)**. The water system is subdivided into 235 regions based on water basins **(c)**. Climate is considered a single global region **(d)**. [Reprinted under a Creative Commons 4.0 International License (CC BY 4.0) from Calvin, K., et al. 2019. "GCAM v5.1: Representing the Linkages Between Energy, Water, Land, Climate, and Economic Systems," *Geoscientific Model Development* **12**. 677–698.]

high-resolution climate models would require too much computing power for hundreds of years of simulations to generate various future emissions scenarios.

Some respondents noted that BER effectively directs its funded research around model uncertainty, promotes process understanding using observations, and encourages close collaborations between DOE national laboratories and research institutions. Others encouraged BER to further connect modeling and observational communities, as well as communities developing machine-learning approaches and new tools. BER could benefit from a strategic plan that comprehensively extends beyond BER modeling to interface with the U.S. and international ESM community.

5.2.3 Human-Earth System Modeling

Traditionally, human influence over the Earth system and Earth's influence over human systems have been studied separately. However, neglecting the interactions between human and Earth systems can miss important emerging properties, bias projections, and misinform projection-based decisions (Reed et al. 2022). For example, decisions involved in designing a reliable and cost-effective electricity distribution system in a coastal region are influenced by projections of Earth system components (e.g., storm surges), human system components (e.g., population changes), and their interactions (e.g., changes in migration and infrastructure hardening in response to realized and projected hazards; Reed et al. 2022).

BER-supported climate research provides opportunities to improve the analyses and projections of coupled human-Earth systems and their interactions in addition to the physical and biogeochemical systems traditionally included in climate research. Examples of BER-supported human-Earth system research include the development of human system models, the coupling of human system models to ESMs, and the incorporation of human and managed systems within ESMs.

BER has supported innovative research on coupled human-Earth systems with world-renowned researchers and tools. For example, the Global Change Analysis Model (Calvin et al. 2019; see Fig. 5.4, this page) has been used to produce scenarios that provided crucial inputs to the IPCC assessment process (Moss et al. 2010). Another example is the recently established MultiSector Dynamics community of practice, a multidisciplinary collective of university and national laboratory researchers working at the interface of human and natural systems (multisectordynamics.org). BER has the potential to become an international leader in the unique and vital MultiSector Dynamics research area and provide decision-relevant insights by considering model uncertainties. Historically, BER-supported researchers contributed to building and sustaining MultiSector Dynamics and linking it to other fields, but the international presence of these researchers has waned in recent years even though this research area is crucial to determining future international leadership.

Respondents identified several potential opportunities to strengthen human-Earth system modeling:

- Develop strategies to improve predictive understanding of coupled human-Earth systems that include relevant uncertainties and thereby better inform decision-making.
- Recruit personnel representing an expanded range of disciplines (e.g., determine how to attract and retain social scientists beyond the discipline of economics).
- Improve linkages between BER-supported U.S. activities and the international community.

5.2.4 Model Intercomparisons

BER is an international leader in climate model intercomparisons, supporting numerous activities including CMIP, which is arguably the most influential and high-profile model intercomparison activity devised to date (see Case Study: CMIP—Coupled Model Intercomparison Project, p. 73). BER's leadership in this area began in the late 1980s with the first climate model intercomparison, the Atmospheric Model Intercomparison Project (AMIP). Formulated under the auspices of the WCRP, AMIP was run by Larry Gates, the director of the BER-supported Program for Climate Model Diagnosis and Intercomparison (PCMDI) at Lawrence Livermore National Laboratory. Through WCRP, PCMDI organized modeling centers around the world to perform AMIP simulations, which were atmospheric models forced by time-evolving observed sea surface temperatures. PCMDI then collected model outputs and made the data available for analysis by scientists around the world. BER's involvement helped extend climate model intercomparison beyond the United States to lead the world's climate scientists in understanding common behaviors and errors in atmospheric models. This work set a precedent for future decades of ongoing BER leadership in international climate model intercomparisons.

While AMIP compared atmospheric components of climate models, CMIP was formulated to compare global coupled climate models with components of atmosphere, ocean, land, and sea ice. CMIP was established with BER leadership provided by PCMDI and BER-supported scientists in WCRP. It has now evolved, with contributed DOE leadership at various levels, to become the pre-eminent international climate model intercomparison activity and the gold standard of model intercomparisons due to its methodology, infrastructure, and representation of international state-of-the-art climate modeling capabilities.

To facilitate sharing of CMIP output and other data, BER supports the Earth System Grid Federation (ESGF), which provides the climate modeling community with distributed data archiving and access capabilities that replace data sharing formerly achieved by shipping data tapes to PCMDI. BER also continues to support model and data evaluation through the PCMDI Metrics Package (PMP) and the Coordinated Model Evaluation Capabilities metrics package. This package includes PMP, the International Land Model Benchmarking (ILAMB) project, and other interagency evaluation packages, thereby enabling comprehensive and holistic evaluations of ESMs.

The model intercomparison landscape is changing as more modeling groups and climate scientists around the world perform intercomparisons not only under the CMIP umbrella but also in stand-alone intercomparisons led by individual research communities.

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CASE STUDY

CMIP—Coupled Model Intercomparison Project

The Coupled Model Intercomparison Project (CMIP) is the most prominent and significant international model intercomparison project devised to date. It has achieved far-reaching success in the international climate science community thanks to support and leadership from BER.

Takeaway

BER support of and leadership in CMIP has been vital to the project's far-reaching success in the international climate science community.

Global climate models that realistically couple atmospheric components with ocean, land, and sea ice components first began to emerge in the 1980s. In 1989, climate scientist Larry Gates established and became the first director of the BER-supported Program for Climate Model Diagnosis and Intercomparison (PCMDI) at Lawrence Livermore National Laboratory to help standardize the field of climate modeling. As a pioneer in his field, Gates was selected to chair a World Climate Research Programme (WCRP) committee that formed a panel to run the new CMIP endeavor. Two BER-supported scientists were among the five members of the first CMIP Panel, and the panel organized the first international workshop on global coupled climate modeling in 1994. The outcome of the workshop was the first phase of CMIP (CMIP1) in 1995 and the second phase, CMIP2, in 1997.

PCMDI established an early international leadership role in CMIP by collecting model outputs from modeling centers and making those data available for analysis by scientists around the world. It also analyzed multimodel datasets and formulated new metrics to evaluate model simulations. Scientific papers emerging from these analyses by DOE-supported scientists and others internationally underpinned key elements of the 2001 Intergovernmental Panel on Climate Change (IPCC) Third Assessment Report.

With continued BER leadership, CMIP3 took model intercomparison to the next level beginning in 2003 with an unprecedented set of coordinated climate change experiments performed by 16 modeling groups from 11 countries using 23 models. PCMDI archived an astounding 31 terabytes of model data made freely available to the international scientific community. Data were accessed via the Internet by more than 1,200 scientists who produced hundreds of scientific papers. The CMIP3 multimodel dataset and associated papers comprised the foundational elements of the 2007 IPCC Fourth Assessment Report and contributed to the awarding of the 2007 Nobel Peace Prize to IPCC science teams.

CMIP5, approved by the WCRP Working Group on Coupled Modelling (WGCM) in 2008, became the most comprehensive model intercomparison effort yet attempted. It had become clear during CMIP3 that climate change science was undergoing a profound paradigm shift. Scientists were pursuing (1) initialized decadal predictions to study near-term climate change; (2) first-generation Earth system models with a coupled carbon cycle to study long-term feedbacks past mid-century with new mitigation scenarios; and (3) new tangible linkages throughout the climate science community including biogeochemistry, atmospheric chemistry, land surface, climate change impacts, and integrated assessment modeling. Through PCMDI, BER structured distributed access of CMIP model data by designing and formulating the Earth System Grid, which enabled modeling centers to upload their data to publicly accessible servers rather than sending their data to PCMDI. With essential funding from BER, the Earth System Grid ultimately joined international partners to become the Earth System Grid Federation (ESGF), an impressive international effort enabling scientists from around the world to more readily download model data. The hundreds of papers resulting from greater access to this data comprised a central part of the 2013 IPCC Fifth Assessment Report.

In 2013, BER led initial planning for CMIP6, which now included 33 modeling groups from 16 countries and

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CASE STUDY

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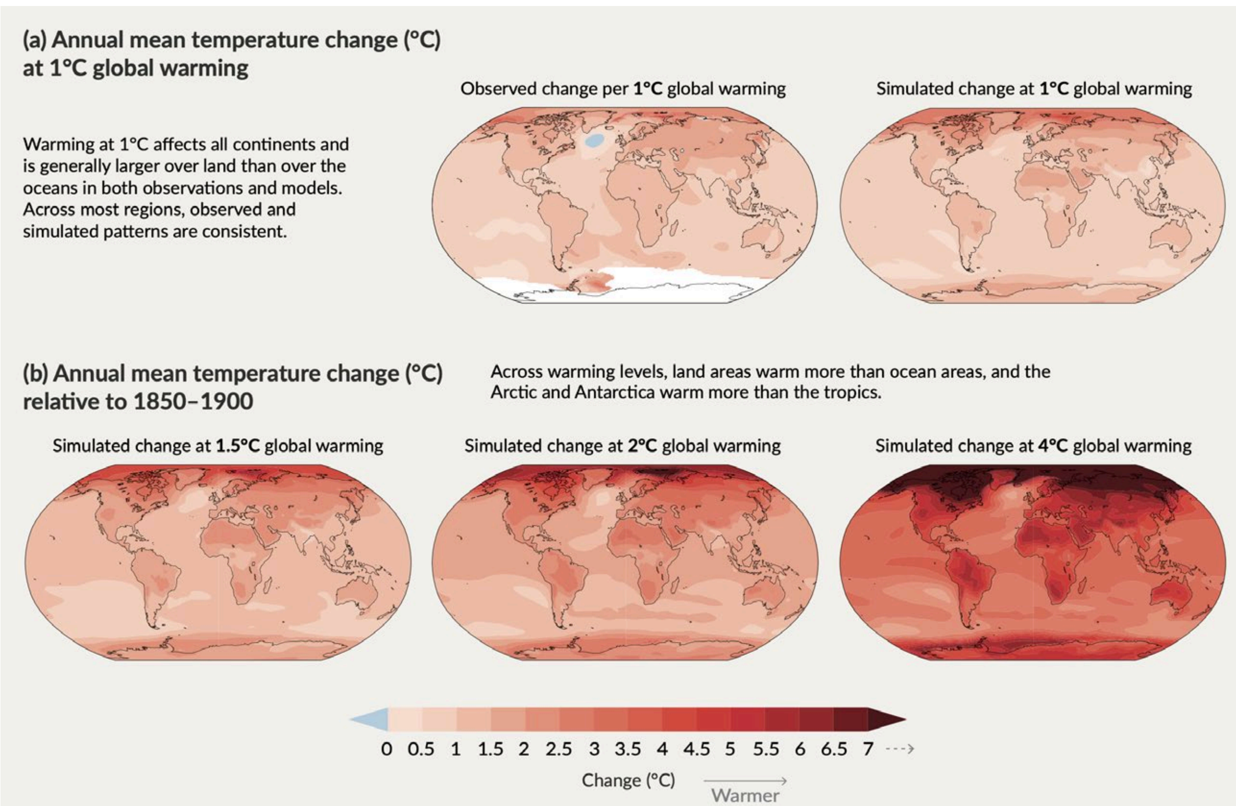
required more formal arrangements for international infrastructure. BER scientists led the WGCM Infrastructure Panel to set standards and policies for sharing climate model output, including establishing input datasets for model intercomparison projects (input4MIPs, esgf-node.llnl.gov/projects/input4mips) to provide boundary conditions and forcing datasets for CMIP6. DOE also provided crucial support for ESGF, the federated data archive hosting CMIP6 data. Model data submitted via ESGF was routinely evaluated using two metrics packages: the DOE-supported PCMDI Metrics Package and the European-based Earth System Model Evaluation Tool.

Similar to previous CMIP phases, thousands of scientists around the world, including DOE-supported scientists at PCMDI and elsewhere, published analyses of CMIP6 model data, which comprised a central element of the 2021 IPCC Sixth Assessment Report (see figure, this page). As with previous IPCC reports, the sixth assessment of future climate change would not have been possible without key leadership from BER-supported scientists in the WCRP-organized CMIP6 model intercomparison activity, an effort that included contributions from modeling groups around the world.



Recent and Future Warming from CMIP6 Models. A key figure from the Intergovernmental Panel on Climate Change *Sixth Assessment Report Summary for Policymakers* shows that changes in regional mean temperature, precipitation, and soil moisture grow larger with each increment of global warming. [Figure SPM.5 from IPCC 2021: Summary for Policymakers. In: *Climate Change 2021: The Physical Science Basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change.* Masson-Delmotte, V., et al. (eds.). Cambridge University Press, Cambridge, UK and New York, NY, USA, pp. 3–32.]

Continued from p. 72

CMIP itself has matured to the point that WCRP established a CMIP Project Office in the United Kingdom to handle CMIP logistics. The Project Office also tracks the growing range of non-CMIP intercomparisons now taking place.

BER and international scientists are broadly engaged in considerable discussion regarding what form CMIP Phase 7 should take, if any. A couple of respondents questioned whether BER should continue to participate in and support CMIP. It is expected that BER will continue to support international model intercomparisons whatever form they ultimately take—by funding either individual scientists or national laboratory groups—because of the significant advancements the work has enabled. CMIP has moved the climate science community firmly into the era of multimodel analyses, and modeling groups gain international visibility and credibility by contributing to comprehensive state-of-the-art datasets. Moreover, analyses of CMIP model data have produced hundreds of scientific papers and advanced the science in ways that complement and provide insights into single-model analyses.

However, separate communities will also likely begin running their own model intercomparisons rather than incorporate their intercomparison activities into the CMIP effort. If this occurs, the model intercomparison effort will become more distributed, but BER can continue its leadership role through PCMDI by tracking intercomparison activities taking place in different communities. BER can also work through WCRP and the CMIP Project Office to participate in and support intercomparison efforts. Certain traditional CMIP simulations may become more operationalized (i.e., simulating historical and future climate change scenarios), but model intercomparisons to study distinct processes and mechanisms in focused disciplinary research communities may achieve greater prevalence scientifically.

Respondents generally concluded that BER-supported scientists should continue to lead international intercomparison activities, including future CMIP phases, as well as intercomparisons organized by individual constituent research communities.

5.2.5 Cloud Feedback and Climate Analysis

BER leads in cloud feedback and climate sensitivity research internationally, as noted by several respondents and as indicated by WCRP reports and IPCC assessment reports on climate sensitivity. Major breakthroughs by BER-supported scientists include understanding cloud feedbacks by decomposing the overall feedback into tangible mechanisms testable by observations (see Case Study: Cloud Feedbacks and Climate Sensitivity, p. 76). BER scientists further developed the concept of emergent constraints to assess aspects of climate feedbacks using observational metrics. The international research community now widely uses the "cloud radiative kernel" technique for quantifying and decomposing cloud feedbacks. BER scientists also pioneered the development and application of instrument simulators to improve comparisons between clouds simulated by climate models and satellite observations.

BER also leads in climate change detection and attribution. BER climate scientists drew from the work of Klaus Hasselmann, a climate modeler and recipient of the 2021 Nobel Prize in Physics, by applying a "fingerprint" method he developed to detect human influence on surface, atmospheric, and ocean temperatures and on different components of the hydroclimate. Their work contributed significantly to advancing the fingerprint research. Continued support for cloud feedback and climate sensitivity research will enable BER to maintain its leadership position in these areas.

5.2.6 Enabling Capabilities

BER climate science includes research and development of enabling capabilities and technologies that support climate research. Enabling capabilities include next-generation computing, artificial intelligence and machine learning (AI/ML), and data assimilation. DOE leads in the development of climate model codes for next-generation computers in the United States,

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CASE STUDY

Cloud Feedbacks and Climate Sensitivity

Takeaway

BER is a world leader in understanding how clouds affect Earth's energy budget, how and why their properties shift under climate change, and how sensitive Earth is to carbon dioxide.

BER-funded scientists have driven major efforts to understand how clouds affect Earth's energy budget, how and why cloud properties respond to climate change, and how sensitive Earth is to carbon dioxide. These accomplishments, outlined below, have advanced international efforts to constrain climate models and quantify Earth's equilibrium climate sensitivity (ECS).

Novel Techniques Developed for Quantifying Cloud Feedbacks and Revealing Underlying Causes

One example is the "cloud radiative kernel" technique used to quantify the sensitivity of top-of-atmosphere radiative fluxes to cloud fraction perturbations and decomposing cloud feedbacks into different cloud types (Zelinka et al. 2012a,b; 2013). This method quickly gained attention in the climate science community and has been cited over 600 times (Google Scholar 2/21/2022). Results from these papers featured prominently in "Chapter 7: Clouds and Aerosols" of the Intergovernmental Panel on Climate Change (IPCC) working group report "AR5 Climate Change 2013: The Physical Science Basis" (Boucher et al. 2013). In partial recognition of this work, DOE atmospheric scientist Mark Zelinka of Lawrence Livermore National Laboratory received the 2022 American Meteorological Society's Henry G. Houghton Award for "innovative advances in understanding the critical involvement of clouds to achieve a better understanding of climate interactions."

Cloud Feedbacks Decomposed into Tangible Mechanisms Testable by Observations

This breakthrough in understanding cloud feedbacks was achieved using so-called "emergent constraints" (Klein and Hall 2015). Emergent constraints are physically explainable empirical relationships between characteristics of the current climate and the long-term climate prediction that emerge in collections of climate model simulations (Klein and Hall 2015). Confirmed emergent constraints identify the areas of a model's simulation of the current climate that are most important for future climate predictions, and they suggest potentially observable predictors that might constrain model predictions. BER scientists recently used this approach to estimate observationally constrained near-global marine low cloud feedback, finding that it is positive but not as large or uncertain as previous estimates (Myers et al. 2021).

Emergent Constraints Applied to Assess Aspects of Climate Feedbacks Using Observational Metrics

DOE scientists Stephen Klein and Mark Zelinka led a recent review article for the World Climate Research Programme (WCRP) assessing the science surrounding how much the Earth will warm in response to a doubling of carbon dioxide (Sherwood et al. 2020). The two led an international group in assessing process evidence from satellite observations, global climate models, large-eddy simulations, and theory to produce a new estimate of Earth's climate sensitivity. The estimate, when combined with estimates from historical warming since the late 1800s and paleoclimate, narrowed the range of Earth's equilibrium climate sensitivity from the often-quoted range of 1.5 to 4.5 kelvins to a likely range of 2.6 to 3.9 kelvins (see figure, p. 77). The researchers' progress on this longstanding issue earned the article runner-up for Science Magazine's 2020 Breakthrough of the Year, as reported in the brief article "Global Warming Forecasts Sharpen" (Voosen 2020). The new analysis provides a better constraint for climate models and served as a key input for the climate sensitivity portion of the IPCC Sixth Assessment Report.

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CASE STUDY

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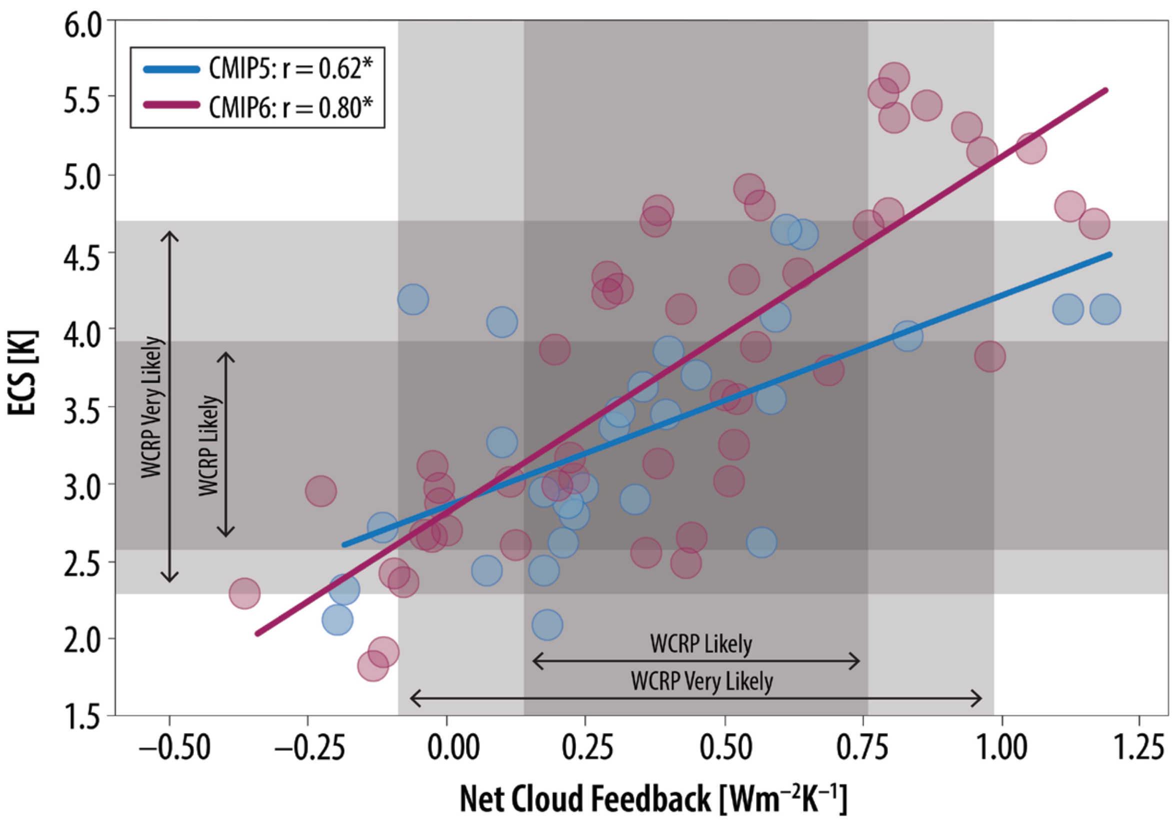
Increased Climate Sensitivity Predicted by Newest Earth System Models

A recent study led by BER scientists determined that the latest generation of global climate models used in the Coupled Model Intercomparison Project predicted greater warming in response to increasing carbon dioxide than previous models (Zelinka et al. 2020). The researchers pointed to changes in how clouds responded to temperature shifts as the primary cause. Specifically, the newer models predicted a greater decline in water content and areal coverage of low-level clouds with greenhouse warming, causing enhanced planetary absorption of sunlight. This important finding was featured in a research spotlight in the science news magazine *Eos* (Shultz 2020). The work was also prominently featured in "Chapter 7: The Earth's Energy Budget, Climate Feedbacks, and Climate Sensitivity" in the IPCC working group report "AR6 Climate Change 2021: The Physical Science Basis" (Forster et al. 2021). The study has been cited over 400 times, earning it recognition from the prestigious *Geophysical Research Letters* journal and ranking it among the top 0.1% of papers in geosciences in the last 2 years by Web of Science.



Improved Climate Models Narrow Earth's Range of Climate Sensitivity. Equilibrium climate sensitivity (ECS) scattered against net cloud feedback for the Coupled Model Intercomparison Project 5 (CMIP5, blue) and CMIP6 (magenta) models. Asterisks indicate across-model correlations that are statistically significant at 95% confidence. Overlain shading indicates the very likely (90%) and likely (66%) confidence intervals of total cloud feedback and ECS. [Courtesy Lawrence Livermore National Laboratory; for more information, see Zelinka et al. 2020. "Causes of Higher Climate Sensitivity in CMIP6 Models," *Geophysical Research Letters* **47**(1), e2019GL085782.]

Continued from p. 75

which is a major investment that other national centers cannot easily attempt. However, a couple of respondents stated that DOE exascale computing is not yet fully realized in E3SM development.

With respect to AI/ML, DOE led a large workshop in 2021 and has the potential to lead especially in applications to climate modeling and integrating observations and models (ai4esp.org/workshop). Despite this potential and the presence of U.S.-based AI/ML experts, several respondents noted opportunities for strengthening these enabling capabilities, including (1) better integrating these efforts into BER climate science, (2) establishing more leadership, and (3) better tailoring some aspects of DOE funding to support "blue sky" research and innovation at national laboratories in a manner that is designed to further the well-defined long-term capabilities that DOE already supports.

Respondents identified data assimilation as a potential gap in DOE capabilities because it is critical to achieving a digital twinning of Earth, or the creation of a dynamic digital replica that accurately mimics the near-term evolution of Earth's relevant systems from their initial state. Data assimilation, which is already used in NOAA weather forecasting and NASA predictive global modeling, offers improved initial conditions for forecasting using high-resolution ESMs and systematically confronts ESMs with observations, thereby providing a powerful tool for identifying model errors.

5.3 Collaboration

5.3.1 Domestic Collaboration

BER impacts climate science at the national level and is generally well connected to universities and other U.S. agencies via its funding mechanisms. However, many interviews with scientific experts and responses to a Request For Information noted a need for increased domestic collaboration. As one international scientist noted, if the United States combined its intellectual and computing capabilities, then no other country likely would be able to compete; however, dispersing climate science across multiple U.S. agencies with relatively weak collaboration enables many international efforts to be competitive. Another respondent noted that multiple agencies working on the same problem could be a strength, enabling independent and unique approaches to the same problem; however, this would also require a mechanism for interagency collaboration to avoid duplication of efforts. Specific areas where improved domestic collaboration may prove beneficial include:

- **Observations**. DOE leads in ground-based observations through ARM, but collaboration is needed to integrate satellite-based observations and to support a digital twin approach to high-resolution global forecasting.
- **Human Systems Data**. BER, through the Multi-Sector Dynamics program, funds research on human impacts to the Earth system, but quality data on human systems is often lacking. Collaborations with social scientists could improve data quality.
- **Modeling**. Duplicative research efforts occur across U.S. agencies, especially in Earth system modeling. Respondents stopped short of recommending a merger of all efforts but did recommend developing a concrete plan for collaboration in the near future between modeling centers to avoid duplication of expense and effort and to increase collective impact.
- **Decision-Making**. DOE funds fundamental science relevant to decision-makers, as do many other agencies. BER's maximum impact depends on effective collaboration with other federal agencies, particularly those with a mandate for developing applied models and research (e.g., U.S. Environmental Protection Agency, U.S. Geological Survey, NOAA, and the U.S. Army Corps of Engineers), to inform management decisions.

Finally, in addition to increasing collaboration across agencies, several respondents noted a need for improved integration across DOE laboratories and between national laboratories and university teams.

5.3.2 International Collaboration

Respondents view international collaboration and leadership as a key measure of success. BER's leading

Fig. 5.5. The Global Reach of DOE's Atmospheric Radiation Measurement (ARM) User Facility. ARM fixed sites and mobile facility deployment locations have spanned all continents, simultaneously relying on and furthering a legacy of international collaboration in climate science and observations. [Courtesy ARM]

roles in IPCC assessments and on science-defining boards, such as the WCRP's, are landmarks in this regard (see Section 5. 1, p. 65).

BER leads internationally in ground-based observations, notably through the ARM program, which excels at the intersection of ground-based measurements and field campaigns (see Fig. 5.5, this page). ARM facilities are in high demand, and the international community often adds its own funding support and participation to ARM-initiated efforts (see Ch. 8: Strategies for People, Partnerships, and Productivity, p. 122). BER could improve international collaboration in this area by supporting the international community's efforts to integrate ground-based climate-observing system datasets.

In terms of Earth system modeling, BER leads internationally in integrating human-Earth system modeling. Respondents suggested that BER consider re-engaging in an integrated assessment modeling consortium, strategically develop its World Bank partnership, and partner with relevant collaborative projects funded by the European Union. BER leads in high-resolution climate modeling at the national level and stands among the leading centers at the international level thanks to extensive computational resources. International collaboration could build on shared computing resources.

BER has a legacy of international leadership in model intercomparison efforts (see Section 5.2.4, p. 72) and now partners with WCRP in the recently instituted

CMIP Project Office in the United Kingdom. The United States (but not yet BER) leads in applying AI/ML methods in modeling. Despite its excellence in process understanding (e.g., aerosol and cloud physics), BER does not yet lead in laboratory studies, which are a third pillar of climate science alongside observations and modeling. A renewed researcher exchange program could enable better integration with other international leaders, providing opportunities for BER-supported researchers to spend time at outstanding partner institutions worldwide and vice versa.

5.4 Future Opportunities

The BERAC subcommittee evaluated BER's international leadership status in climate science based on the program's roles in major international science committees, its contributions to the IPCC assessment process, and its national and international influence on climate research and similar programs.

For IPCC assessment reports, BER-supported research has contributed significantly. In terms of climate science contributions, feedback received from interviews and responses to the Request For Information indicated that BER leads internationally in many research areas. These areas include: (1) climate analyses encompassing cloud feedbacks, climate sensitivity, and attribution and detection of climate change; (2) process understanding of aerosols and clouds and their interactions; (3) Earth system modeling coupled with human-Earth system modeling; (4) global ground-based observations and associated field campaigns; and (5) climate model intercomparisons, including CMIP, the most influential and high-profile model intercomparison activity.

Continued strong support for these established international leadership areas is crucial to BER maintaining its capacities to lead. In addition, opportunities for increased leadership are outlined below in the following topical areas: high-resolution Earth system modeling, coupled human-Earth system modeling, ARM and ASR, international model intercomparisons and climate analysis, and funding modalities.

5.4.1 High-Resolution Earth System Modeling

BER uses high-performance DOE computing capabilities to perform cutting-edge research on developing a kilometer-scale ESM (see Fig. 5.6, p. 81). BER's initial success with the E3SM 3-km convection-permitting model positioned BER ahead of other U.S. contributors and among several world leaders in the field. BER also has potential to lead in the application of AI/ML approaches, particularly with respect to climate modeling and integrating observations and models. Collaboration with existing U.S. leaders and integration with interagency climate science are critical for BER to establish such leadership. Beyond AI/ML applications, BER could foster innovation in several areas by enabling small-group and principal investigator–driven research in higher-risk and higher-payoff areas. Given DOE's unique strength in computing, BER should continue to pursue high-resolution modeling efforts, ideally in collaboration with other U.S. modeling centers to avoid duplicative efforts and maximize scientific advances. Considering limited resources, BER may want to focus on developing the kilometer-scale E3SM model because the higher resolution encourages improved interagency collaboration around satellite remote-sensing data (with NOAA and NASA), which could become crucial if a digital twin approach is pursued (see Ch. 7: Integrative Science, p. 103).

5.4.2 Coupled Human-Earth System Modeling

BER is perceived as a natural home for developing capabilities in crosscutting research encompassing energy-related studies and human-Earth system modeling. Whereas BER historically led the field, European groups have recently caught up or surpassed U.S. capabilities. Politics may have negatively impacted U.S. ability to maintain consistent leadership in the field internationally. A plan to transition research-grade human-ESM forecast models to deliver operational products to public and private stakeholders, similar to weather and seasonal forecasts, could help offset politicization, as discussed further in Ch. 7: Integrative Science, p. 103. BER has the potential to lead internationally in providing decision-relevant insights

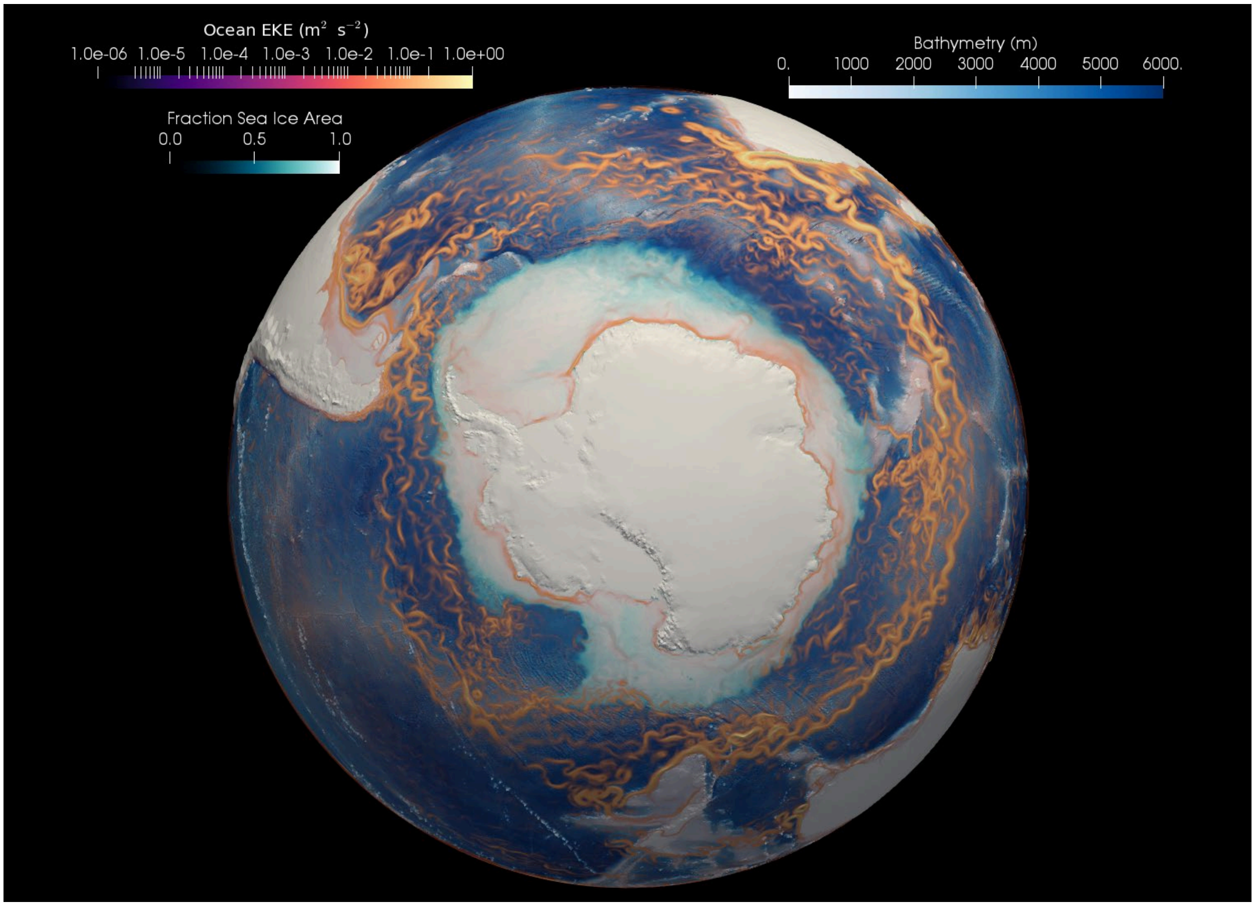


Fig. 5.6. Modeling Earth Systems in High Resolution. The Energy Exascale Earth System Model (E3SM) uses exascale computing to carry out high-resolution Earth system modeling of natural, managed, and man-made systems to answer pressing problems in DOE mission areas. This image from a high-resolution E3SM simulation shows sea-ice extent (bluish-white) around Antarctica (center) and oceanic currents associated with strong mesoscale eddy activity (orange). These currents play an important role in transporting heat from warmer mid-latitudes to Antarctica, where it can melt ice shelves. [Courtesy Los Alamos National Laboratory]

considering model uncertainties by improving predictive understanding of the coupled human-Earth system.

5.4.3 ARM and ASR

The combination of BER's ground-based measurement capabilities and field campaign support sets world standards, but the European community has now integrated a wide array of previously unaffiliated ground sites and lifted standards in some operational respects. Going forward, domestic and international ground site networks should adopt shared data quality standards and collectively deposit their historical and future data into shared databases. A stronger strategic plan could also better integrate ARM observations with ESM development, perhaps spanning E3SM and the U.S. Earth system modeling community within the context of a nationally integrated effort (see Ch. 7: Integrative Science). Finally, BER could consider establishing a major laboratory chamber user facility for cloud and aerosol research in the United States, on a par with modern European facilities. DOE laboratories offer the most appropriate environment and already house the greatest concentration of relevant expertise domestically. A history of international exchange opens the possibility of BER drawing upon existing European designs and lessons learned.

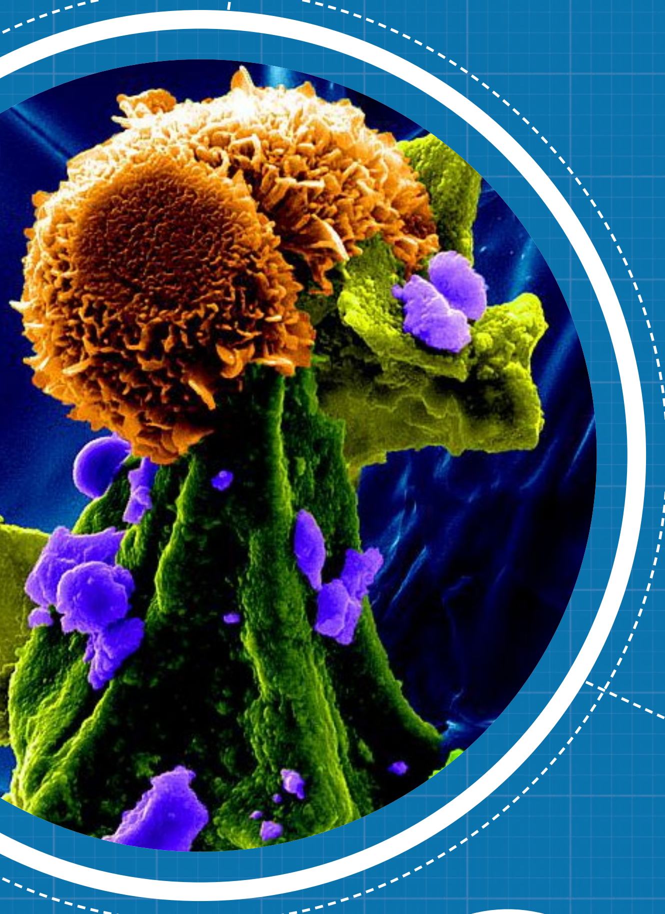
5.4.4 International Model Intercomparisons and Climate Analysis

A key aspect of BER's international leadership is its role in leading and participating in model intercomparisons such as CMIP. BER also leads in cloud feedback and climate sensitivity research, according to WCRP reports and IPCC assessment reports. BER is encouraged to continue to work through PCMDI to conduct international model intercomparison activities involving both future CMIP phases and intercomparisons organized by individual research communities. DOE's support of ESGF for CMIP data distribution and the Coordinated Model Evaluation Capabilities metrics package, which includes PMP, is critical to maintain BER leadership in multimodel diagnostics and evaluation, areas where BER could be outmoded by the European-based Earth System Model Evaluation Tool. Continuous support for cloud feedback and climate analysis research is also required to ensure BER's scientific leadership.

5.4.5 Funding Modalities

BER advances its mission areas via support for user facilities, Science Focus Areas at DOE national laboratories, and grants to domestic and international research entities external to DOE. The SFA process supports development of long-term capabilities while retaining flexibility to adjust course, but it lacks emphasis on discovery research at a small scale within laboratories. Adding a small-scale proposal-driven funding modality would provide two key advantages. First, it would allow scientists an additional avenue to participate in career-defining work of their own design, which is the norm within the wider research community, thus increasing engagement and reward. Second, seeding a diversity of high-risk, high-return ideas increases innovation. For example, the operation of discovery or blue sky grants within climate science could accelerate AI/ML applications. Another shortfall of the SFA process is the barrier it presents to funded collaboration between BER researchers and external entities. This prevents the efficient importation of expertise to fill knowledge gaps or share lessons learned. Within ESM development, collaborative engagement can accelerate learning and prevent shortfalls of model performance where expertise may be lacking. Other U.S. agencies experience similar barriers for similar reasons. BERAC recommends addressing this problem more boldly in the field of climate science and establishing sustained, substantial funding streams to support expanded collaboration with U.S. agencies and universities to improve research outcomes and ensure integration of efforts to meet societal needs.

CHAPTER 6
Enabling Infrastructure



Working Group Co-Leads

Kerstin Kleese van Dam, *Brookhaven National Laboratory*
Robert F. Fischetti, *Argonne National Laboratory*

Working Group Members

Kenneth James Davis, *The Pennsylvania State University*
Ben Evans, *Australian National University*
Serita Frey, *University of New Hampshire*
Thomas R. Schneider, *European Molecular Biology Laboratory, Germany*

Chapter 6
Key Finding and Recommendations

Key Finding

KF6.1 The review showed that BER research is currently supported by six world-class infrastructure capabilities:

a. **DOE Joint Genome Institute (JGI).** BER's JGI is the world's largest center for nonbiomedical genomic science research, supporting DOE missions in clean energy and environmental characterization and cleanup. It provides integrated high-throughput sequencing and computational analysis that enable systems-based approaches to these challenges.

b. **Atmospheric Radiation Measurement (ARM) User Facility.** BER's ARM is internationally recognized for its long-term ground-based observation facilities, which have been advancing global atmospheric and climate research for 40 years. ARM's long-term data records, breadth of conditions and locations over diverse climate-relevant areas, and influence in the study of the climate system are unmatched by any other ground-based programs around the world.

c. **AmeriFlux and the AmeriFlux Management Project.** BER-supported AmeriFlux is a collection of long-term, eddy flux stations that measure ecosystem carbon, water, and energy fluxes across the Americas. One of two leading global flux networks, AmeriFlux is part of the international FLUXNET project and has taken the lead in creating the FLUXNET synthesis data products, the most impactful international observational product.

d. **National Synchrotron Light Source II (NSLS-II).** Supported by DOE's Office of Basic Energy Sciences, NSLS-II is the newest and most advanced synchrotron in the United States. The facility's design optimizes the creation of tightly collimated, high-flux light beams, covering the spectral range from infrared to high-energy X-rays. This unique combination of performance characteristics has allowed the creation of world-leading instruments, such as imaging with high spatial resolution (~10 nm) and chemical sensitivity, opening up novel possibilities for the study of biological material dynamics. Additional BER co-funded instruments with small beams (1 µm) are enabling high-resolution structural information from tiny protein crystals.

e. **DOE Leadership Computing Facilities.** Supported by DOE's Advanced Scientific Computing Research program, the Argonne Leadership Computing Facility, Oak Ridge Leadership Computing Facility (OLCF), and National Energy Research Scientific Computing Center are critical parts of the enabling infrastructure on which BER scientists rely. In June 2022, the high-performance computing community's international benchmarking effort ranked OLCF's Frontier supercomputer as the fastest in the world after it became the first system to break the exascale barrier. What distinguishes these DOE systems from international comparators is the science support ecosystem around them, provided by the DOE Exascale Computing Project (ECP). BER science has benefited from ECP in both its climate (Energy Exascale Earth System Model) and biology (ExaBiome) research.

f. **Environmental Molecular Sciences Laboratory (EMSL).** EMSL delivers leading facilities, advanced instrumentation, and scientific leadership that empower and enable a national and international community of researchers to advance BER's mission to achieve a predictive understanding of complex biological, Earth, and environmental systems.

Recommendations

R6.1 Establish an oversight board to assess strategic decisions about creating, continuing, and sunsetting all BER infrastructure capabilities. This board should develop and publish a regularly updated 5- to 10-year strategic roadmap for infrastructure capabilities that support mission-critical science, coordinating with other DOE offices and national and international agencies to maximize investment and impact.

R6.2 Promote greater integration across user facilities—including harmonization of data management and analysis services—to enable researchers to easily schedule and use different infrastructure capabilities.

R6.3 Consider creating data user facilities and providing long-term support for their governance, planning, policy development, and technological needs.

R6.4 Establish a cross-facility working group to develop and share a foundational BER data policy and best practices for data use, licensing, and citation.

R6.5 Increase computational and storage capacity for BER researchers.

6 Enabling Infrastructure

6.1 Overview of Enabling Infrastructure Facilities and Services for BER Science

Diverse DOE experimental, observational, and computational user facilities and services play critical roles in supporting a broad national and international user community engaged in BER science, missions, and major scientific achievements (see Fig. 6.1, this page). This chapter describes and reviews the international competitiveness of these resources, specifically 15 DOE capabilities, six of which are world leaders (see Fig. 6.2, p. 86). BER science also significantly relies on institutional laboratory and computational resources, and a more detailed study assessing their competitiveness could be helpful in the future but is beyond the scope of this report.

These user facilities and services have enabled scientific breakthroughs in BER genomic and climate science for decades, and their impact is evident in groundbreaking research, including Nobel Prize–winning studies. Moreover, in times of national crisis, BER's enabling infrastructure plays a key role in DOE's response. For example, during the COVID-19 pandemic, BER's biological systems science infrastructure provided critical capabilities to large teams of multidisciplinary scientists assembled as part of DOE's National Virtual Biotechnology Laboratory (NVBL).

6.1.1 Infrastructure-Supported Advances in Genomic Science

1985 to 2001

The Human Genome Project (HGP) remains one of the most successful multi-institutional international science efforts in history (IHGSC 2001). In 1997, DOE created the Joint Genome Institute (JGI) to unite the sequencing and informatics expertise at several DOE national laboratories and accelerate the

Fig. 6.1. BER Infrastructure Supporting National and International Science. This map shows the institutions of scientists using BER user facilities in 2020. [DOE Office of Science]

DOE Enabling Infrastructure Capabilities

Biological Systems Science

BER user facilities and project-based community services

- Joint Genome Institute, *jgi.doe.gov*
- Systems Biology Knowledgebase (KBase), *kbase.us*

Basic Energy Sciences or non-designated user facilities with BER-funded capabilities in structural biology and imaging

- Advanced Light Source, *als.lbl.gov*
- Advanced Photon Source, *aps.anl.gov*
- National Synchrotron Light Source II, *www.bnl.gov/nsls2/*
- Spallation Neutron Source and High Flux Isotope Reactor, *neutrons.ornl.gov/sns* and *neutrons.ornl.gov/hfir*
- Stanford Synchrotron Radiation Lightsource, *www-ssrl.slac.stanford.edu*
- Laboratory for BioMolecular Structure, *www.bnl.gov/cryo-EM/*

Earth and Environmental Systems Sciences

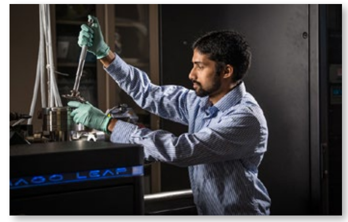
BER user facilities and project-based community services

- Atmospheric Radiation Measurement Research user facility, *www.arm.gov*
- Earth System Grid Federation, *esgf.llnl.gov*
- Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE), *ess-dive.lbl.gov*

Community services with partial BER support

- AmeriFlux, *ameriflux.lbl.gov*

Crosscutting



BER's Environmental Molecular Sciences Laboratory user facility

www.emsl.pnnl.gov

Advanced Scientific Computing Research user facilities for high-performance computing

- National Energy Research Scientific Computing Center, *www.nersc.gov*
- Argonne Leadership Computing Facility, *www.alcf.anl.gov*
- Oak Ridge Leadership Computing Facility, *www.olcf.ornl.gov*

Fig. 6.2. BER Enabling Infrastructure. The BER community is supported by 15 enabling capabilities stewarded by BER, the Basic Energy Sciences program, and the Advanced Scientific Computing Research program. [Courtesy DOE Joint Genome Institute, Argonne National Laboratory, DOE Atmospheric Radiation Measurement user facility, AmeriFlux/John Knowles, Environmental Molecular Sciences Laboratory, Oak Ridge National Laboratory, and Energy Exascale Earth System Model project]

HGP's completion. By project's end, not only had scientists sequenced the full human genome, but the resulting advances in genomic sequencing technology set in motion a revolution in biotechnology and genomic science that continues to this day.

2016
JGI capabilities in environmental metagenomics enabled unprecedented insights into the composition and functioning of whole microbial communities controlling carbon and nutrient cycling in the environment. Researchers recovered thousands of complete microbial genomes through terabase-scale (10^{12} DNA bases), cultivation-independent metagenomic sequencing of an aquifer sediments community (Alivisatos et al. 2015; Bendall et al. 2016; Eloe-Fadrosh et al. 2016; Markowitz et al. 2015; Nagy et al. 2015; Olsen et al. 2016; Oyserman et al. 2016; Pernice et al. 2015; Solomon et al. 2016).

2017
JGI users successfully adapted a yeast DNA recombination system to engineer two entire pathways into a plant: a soil bacterial pigment and a biodiesel metabolic pathway. By radically simplifying the stacking of genes from multiple sources and engineering them into a different organism, this work significantly advances the development of new biotechnology tools for a broad range of plants (Dossani et al. 2017).

2019
At the Environmental Molecular Sciences Laboratory (EMSL), a team of university scientists produced a three-dimensional map of the metabolic products from bacteria found in root nodules. Using EMSL's high-field Fourier transform ion cyclotron resonance mass spectrometers, the team visualized metabolites colocated in different nodule compartments. This spatial perspective will help unravel the complexity of these highly interdependent microbes, optimize crop production, and enable more sustainable agricultural practices for global food crops (Liu et al. 2020).

6.1.2 Infrastructure-Supported Advances in Climate Science

2011
By analyzing observed and model-simulated extreme precipitation over North America from 1951 to 1999, BER-funded scientists produced the first conclusive evidence that human-induced increases in greenhouse gases intensify heavy precipitation events (Min et al. 2011).

2014 to 2015
A collaboration between the United States and Brazil used the Atmospheric Radiation Measurement user facility (ARM) to discover key factors affecting cloud and precipitation patterns in the Amazon Basin. The team found that aerosol concentrations that modulate these patterns are maintained by vertical transport from the lower troposphere in convective downdrafts. Furthermore, researchers demonstrated that widespread biases in climate model simulations of daily and seasonal water cycles over the Amazon are attributable to inaccurate model representations of the ubiquitous fog that forms within the forest canopy, which is responsible for a significant regional cloud-albedo feedback. These findings are critical for generating better predictions of climate change in the tropics (Anber et al. 2015; Wang et al. 2016).

2015
Scientists used ARM observational data and measurements to compute for the first time the extent to which rising greenhouse gas concentrations have altered Earth's surface radiative balance. The researchers analyzed 10 years of coincident carbon dioxide (CO_2) concentrations and the spectrum of downwelling infrared radiance at ARM observatories in Alaska and Oklahoma. Their results confirmed predictions that rising CO_2 concentrations have led to increases in clear-sky surface radiative forcing of 0.2 W/m^2 per decade at mid- and high latitudes. These findings provide irrefutable evidence that rising greenhouse gases are altering the climate's radiation balance (Feldman et al. 2015).

2022
Researchers used long-term AmeriFlux observations of carbon cycling between ecosystems and the atmosphere to detect, for the first time, increasing photosynthetic CO_2 uptake due to the fertilization effect of rising atmospheric CO_2 concentrations (Chen et al. 2022). These results demonstrate the utility of long-term measurement networks, such as those supported by DOE's AmeriFlux Management Project,

for observing ecological responses to anthropogenic changes in Earth's atmosphere.

6.2 Indicators of Leadership

The enabling infrastructure for BER science offers a broad range of capabilities, some of which are world leading and detailed herein. However, all these services and facilities are facing robust international competition to meet increasing compliance related to scientific citation, publishing, and technology offerings. BER will need to make targeted investments to keep these resources at the forefront.

The BERAC subcommittee used the following metrics to assess the leadership of specific facilities:

- Ability to enhance and support the scientific community's research efforts, from planning to execution to publication.
- Sufficient availability of quality infrastructure capabilities to enable access for most researchers.
- One or more groundbreaking, transformational, or unique capabilities that give researchers significant advantages in their discovery science.
- For digital archives, adherence to data principles that are FAIR (findable, accessible, interoperable and reusable) and provision of all data needed by the research community.
- Comparison and collaboration with similar international facilities.

Based on these criteria, the subcommittee—following additional discussions with experts—identified six world-class facilities and services: JGI, ARM, AmeriFlux and the AmeriFlux Management Project, National Synchrotron Light Source II (NSLS-II), DOE supercomputing user facilities, and EMSL.

6.2.1 DOE Joint Genome Institute

JGI is the largest genomic science center worldwide for exclusively performing DOE mission-relevant (non-biomedical) genomics research. It fills a critical niche, enabling studies related to the most pressing challenges in energy and environmental research. JGI is unique in offering free access to large-scale data production and cutting-edge genomic capabilities to a global community of users working on DOE mission-relevant scientific questions (see Fig. 6.3, this page). Its sequencing and data infrastructure capacity affords the execution of extremely large studies, such as the 55 trillion basepair switchgrass genome study (Lovell et al. 2021) and the cataloging of 145,439 metagenome-assembled genomes of bacteria and archaea, along with 1,947,640 novel genomes from giant (2,055) and other viruses (1,945,585).

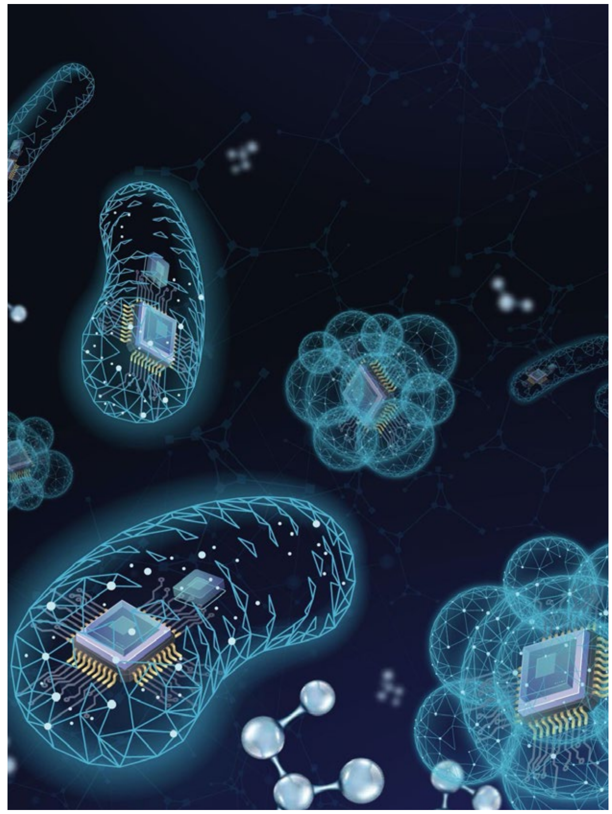


Fig. 6.3. Characterizing Specialized Metabolites. Graphic representation of an important addition to the synthetic biologist's toolkit developed by JGI: a technique for chassis (or strain)-independent recombinase-assisted genome engineering (CRAGE). [Reprinted by permission from Wang, B., et al. 2020. "CRAGE-Duet Facilitates Modular Assembly of Biological Systems for Studying Plant–Microbe Interactions," *ACS Synthetic Biology* **9**(9), 2610–615. ©2020 American Chemical Society.]

No comparable institutions offering services at this scale and exclusively focused on DOE mission-relevant questions exist in the United States or internationally. Although Genoscope, the main sequencing center in France, is also dedicated to environmental sciences, its sequencing capacity is about 10 times lower than JGI's. Genoscope mainly sequences samples from the Tara Oceans project, focusing on marine ecosystems. The German Genome Center also has a much lower sequencing and annotation capacity than JGI. In China, The Beijing Genomics Institute (BGI) has a stronger sequencing capacity, including environmental samples, but the Chinese have not been able to build a community interface, such as JGI's MycoCosm, which targets the large-scale sequencing and analysis of fungal genomes to explore the phylogenetic and ecological diversity of fungi. MycoCosm integrates fungal genomics data and analytical tools, promoting user community participation in data submission, annotation, and analysis.

The only sequencing center comparable to JGI is the Wellcome Sanger Institute in the United Kingdom. For many years, the institute mostly dealt with medical sciences, but the goals of its new Darwin Tree of Life project—to produce "genomic data to understand the evolution of the diversity of life, to explore the biology of organisms and ecosystems, and to aid conservation efforts"—are very similar to JGI objectives (darwintreeoflife.org). JGI currently is a clear leader in its field, but competition from China and the United Kingdom is closing the gap.

6.2.2 DOE Atmospheric Radiation Measurement User Facility

ARM is internationally recognized for its long-term ground-based observation facilities, which have advanced global atmospheric and climate research for 40 years. In addition to fixed sites that provide long-term continuous measurements of radiative fluxes, atmospheric aerosols, clouds, and related atmospheric variables, ARM deploys mobile ground facilities to diverse climate regimes around the world and operates a dedicated aerosol facility for process studies and atmospheric and climate model improvements. ARM's long-term data records, breadth of conditions and locations, and influence in climate system research are unmatched by any ground-based program worldwide. ARM's sophisticated suite of measurements at its fixed and mobile facility sites also sets a standard for other climate-observing facilities.

In 2000, the European Union established the Aerosol, Clouds, and Trace Gases Research Infrastructure (ACTRIS), which integrates and leads atmospheric observation capabilities across 22 European countries and more than 100 organizations, including prior existing facilities such as EUSAAR (European Supersites for Atmospheric Aerosol Research). ACTRIS research is focused on vertical aerosol distribution, *in situ* aerosol properties, trace gases, and cloud observations and includes a significant modeling component. The distributed ACTRIS network seeks to engage member-country resources as diverse as laboratory chambers and unmanned aerial vehicles. In contrast, ARM supports, under a single umbrella, an extensive range of field campaign activities through its fixed and mobile site deployments, often collaborating closely with other U.S. agencies and international partners (see Ch. 5: Climate Science, p. 63).

Although not as established as ARM, ACTRIS has impressive publication, data download, and user numbers, and its funding support and economies of scale have enabled unique calibration facilities. ARM may already require some new investments to match ACTRIS's long-term measurement quality. ACTRIS is now the long-term ground-based measurement program to keep pace and collaborate with in order to deliver well-calibrated, long-term, ground-based atmospheric measurements to international databases.

6.2.3 AmeriFlux and the AmeriFlux Management Project

AmeriFlux is a collection of long-term, eddy flux stations that measure ecosystem carbon, water, and energy fluxes across the Americas. One of two leading global flux networks, AmeriFlux is part of the international FLUXNET project and leads the creation of the project's globally impactful synthesis data products.

AmeriFlux's open data policy has a strong positive impact on the global flux network. The AmeriFlux Management Project (AMP) has led multiple important international synthesis studies. The 2021 Sixth

Assessment Report of the Intergovernmental Panel on Climate Change cites FLUXNET, the FLUXNET2015 dataset (produced by AMP), and, in particular, the availability of more than 20 years of site data records (supported through the AMP Core site program) among the major developments in the expansion of observational capacity of the atmosphere, land, and hydrological cycle. AmeriFlux cross-site calibration facilities are world-leading. Their lack of standardization relative to Europe's Integrated Carbon Observation System (ICOS) and the National Science Foundation's National Ecological Observatory Network (NEON) is a strength, allowing AmeriFlux sites to quickly adapt to shifting research priorities and support a wide range of experiments. For example, ICOS is more integrated with other observing systems but focused entirely on carbon. AmeriFlux is both broader—encompassing all ecosystem-atmosphere fluxes—and narrower because it is not integrated with atmospheric carbon measurements such as those collected by the National Oceanic and Atmospheric Administration (NOAA).

6.2.4 National Synchrotron Light Source II

NSLS-II is the newest and most advanced synchrotron in the United States. Its design optimizes the creation of tightly collimated, high-flux light beams that cover the spectral range from infrared to high-energy X-rays. NSLS-II's unique performance characteristics have enabled researchers to develop world-leading instruments and capabilities of interest to the BER research community. For example, coherent X-rays produced at NSLS-II are opening new possibilities for imaging and studying biological material dynamics. A combination of instruments enables imaging with high spatial resolution (~10 nm), chemical sensitivity, and speed at environmental to subcellular scales. These imaging capabilities are currently unmatched, although future upgrades will make both DOE's Advanced Photon Source at Argonne National Laboratory and the European Synchrotron Radiation Facility competitive in the hard X-ray region.

Structural biology research also benefits from NSLS-II's design, leading to best-in-class instruments for macromolecular crystallography and X-ray scattering that are

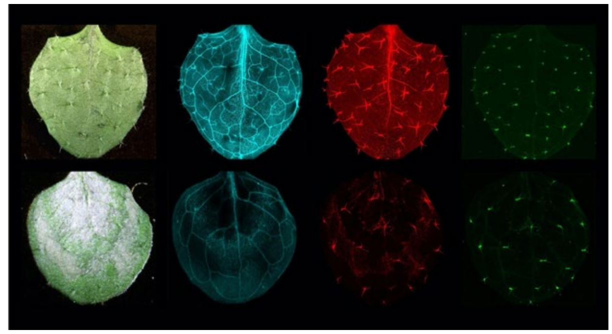


Fig. 6.4. Study Sheds Light on Plant Response to Low Iron. Researchers used X-ray fluorescence imaging techniques at NSLS-II to identify how iron-deficient plants optimize photosynthesis to protect themselves from absorbing too much light. [Reprinted from Akmakjian, G. Z., et al. 2021. "Photoprotection During Iron Deficiency Is Mediated by the bHLH Transcription Factors PYE and ILR3," *PNAS* **118**(40), e2024918118.]

co-funded by BER. Sophisticated automation combined with on-the-fly data analysis is offering scientific insights into the relationship between structure and function, reaction mechanisms, and imaging for novices and experts alike (see Fig. 6.4, this page). These structural biology capabilities are competitive with, if not better than, all other facilities in the world. Their coordination in tackling common scientific challenges will provide an important resource for the BER community for years to come.

6.2.5 DOE Supercomputing User Facilities

Funded by the Advanced Scientific Computing Research (ASCR) program, DOE's three supercomputing facilities—the National Energy Research Scientific Computing Center (NERSC) at Lawrence Berkeley National Laboratory and the leadership computing facilities at Argonne and Oak Ridge national laboratories (ALCF and OLCF)—are unique national resources that support scientific discovery. Although not BER-funded, these user facilities are critical parts of the enabling infrastructure on which BER scientists rely.

Twice a year, the high-performance computing community conducts an international benchmarking effort known as the TOP500 to determine the world's fastest scientific computing systems (TOP500 2022). In

June 2022, OLCF's Frontier supercomputer earned the No. 1 ranking after it achieved an unprecedented level of computing performance known as exascale, a threshold of 1 quintillion calculations per second. Also ranked were OLCF's Summit system in fourth, NERSC's Perlmutter system in seventh, and ALCF's Polaris in fourteenth place.

After decades-long dominance by U.S. systems, Japan and China are catching up in computing size and capacity. However, compared to international competitors, DOE systems have the distinction of a science-support ecosystem provided by the DOE Exascale Computing Project (ECP), which is deploying the applications, software technologies, and hardware needed to ensure scientific impact at the exascale. BER science is benefiting from ECP in two key efforts that will use world-leading exascale computing systems: (1) the Energy Exascale Earth System Model (E3SM), BER's flagship climate modeling code that incorporates the most up-to-date simulation research from U.S. scientists, and (2) the ExaBiome project, which is developing exascale software solutions for analyzing vast troves of metagenomics data to better understand microbiome dynamics, including biogeochemical cycles.

6.2.6 Environmental Molecular Sciences Laboratory

EMSL delivers leading facilities, advanced instrumentation, and scientific leadership that empower and enable a national and international community of researchers to advance BER missions. The facility is supported by a staff of 160 scientists with expertise in the biological, chemical, environmental, computational modeling, and data sciences who continuously develop new methodologies and push the limits of current technologies. EMSL operates more than 150 advanced and often one-of-a kind instruments including high-field *in situ* nuclear magnetic resonance; high-resolution, high-accuracy mass spectrometry (MS); and cutting-edge bioimaging.

No other institution offers such a broad collection of instruments under one roof that can be integrated to solve complex research problems. For example, although the National High Magnetic Field Laboratory (operated by Florida State University, the University of Florida, and Los Alamos National Laboratory) is the world's largest and most powerful magnet laboratory, it lacks EMSL's breadth of instruments and integration with other BER facilities. The European Molecular Biology Laboratory offers a broader spectrum of experimental services, but they are geographically distributed across five sites, making integrated analytics much more difficult. EMSL scientists have incorporated the 21 Tesla Fourier transform ion cyclotron resonance–MS into research for single-cell metabolomic analysis to complement the single-cell sequencing capability at JGI. Another example is the nanodroplet processing in one-pot for trace samples (nanoPOTS) N2 chip that enables high-throughput and high-efficiency sample preparation for single-cell proteomics. This platform can quantify roughly 1,500 proteins from about 100 individual cells from three cell lines. The new workflow (1) eliminates tedious and time-consuming tandem mass tag (TMT) pooling steps, (2) improves sample recovery and proteomics sensitivity, and (3) provides high reproducibility. The new chip and workflow also reduce the processing time from the previous nanoPOTS-TMT workflow by half, while improving the throughput and efficiency of single-cell proteomics (Woo et al. 2021).

A central theme for EMSL is integration across its research platforms. In 2015, EMSL broadened that concept to bridge across BER user facilities. From this idea of cross-facility collaboration came the Facilities Integrating Collaborations for User Science (FICUS) program. Initially a collaborative effort between JGI and EMSL, FICUS represents a unique opportunity for researchers to combine the power of multiple BER user facilities in one proposed research project. After several successful years of EMSL-JGI FICUS calls for proposals, the program has expanded to include ARM, the National Science Foundation's National Ecological Observatory Network, and the Bio-SANS beamline at Oak Ridge National Laboratory's High Flux Isotope Reactor.

6.3 Leadership Status

The BER community is supported by 15 enabling infrastructure capabilities stewarded by BER, the Basic Energy Sciences (BES) program, and ASCR. These capabilities support critical science including Nobel Prize–winning research (see BER-Related Nobel Prize Winners, p. 92). Six of the capabilities are recognized by experts as world-class (see Section 6.2, p. 88). Their

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BER-RELATED NOBEL PRIZE WINNERS

BER science is supported by a wide range of experimental, observational, and computational user facilities and services. These enable the research community to accomplish BER missions, and their impact is exemplified in the role they have played over the years in supporting major scientific achievements, including Nobel Prize–winning research.

2003

Roderick MacKinnon

Nobel Prize in Chemistry

Awarded for work explaining how a class of proteins helps generate nerve impulses — the electrical activity that underlies all movement, sensation, and perhaps even thought. The work leading to the prize was primarily carried out at the National Synchrotron Light Source (NSLS).

2007

- Al Gore
- Intergovernmental Panel on Climate Change

Nobel Peace Prize

Awarded for efforts "to build up and disseminate greater knowledge about man-made climate change, and to lay the foundations for the measures that are needed to counteract such change." IPCC was, and is to this day, heavily reliant on the services of the Earth System Grid Federation (ESGF) to conduct and evaluate its climate modeling scenario analysis.

2009

- Venkatraman Ramakrishnan
- Thomas Steitz
- Ada Yonath

Nobel Prize in Chemistry

Awarded for studies of the structure and function of the ribosome. Macromolecular X-ray protein crystallography experiments at the Advanced Photon Source and NSLS were critical to the success of Ramakrishnan and Steitz's research.

2013

- Martin Karplus
- Michael Levitt
- Arieh Warshel

Nobel Prize in Chemistry

Awarded for developing pioneering methods in computational chemistry that brought a deeper understanding of complex chemical structure and reactions in biochemical systems. To investigate enzyme catalysis mechanisms, research that could not be accomplished experimentally, Karplus turned to the National Energy Research Scientific Computing Center (NERSC) to develop methods to study them computationally.

2017

Joachim Frank

Nobel Prize in Chemistry

Awarded to Frank, a NERSC user and principal investigator, for the development of software used to reconstruct three-dimensional structures of *in situ* biological molecules from transmission electron microscopy images. Frank pioneered the computational methods needed to reconstruct the 3D shape of biomolecules from thousands of 2D images obtained from cryo-EM. These methods are employed today by most structural biologists who use electron microscopy.

2020

- Jennifer Doudna
- Emmanuelle Charpentier

Nobel Prize in Chemistry

Awarded for the "revolutionary impact on the life sciences" resulting from Doudna and Charpentier's development of CRISPR/Cas9 technology. The two partnered with the DOE Joint Genome Institute to use the Integrated Microbial Genomics and Microbiomes system to mine the immense collection of publicly accessible metagenomic datasets from a wide variety of ecosystems around the world, conducting iterative searches using statistical analyses to continuously refine the process of finding novel Cas genes and CRISPR systems.

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available capacity varies, with some facilities, such as JGI and ASCR computing, being vastly oversubscribed.

BER researchers have access to some unique capabilities that can provide a distinct competitive advantage in scientific discovery. Notable among them are JGI's cutting-edge genomic capabilities coupled with leading data analytics and data access support, EMSL's single-cell metabolomic and proteomic analyses, and NSLS-II biological imaging capabilities. Other BER co-funded facilities have played leadership roles in the past decade. The Structural Molecular Biology group at the Stanford Synchrotron Radiation Lightsource championed automation, which increased throughput and enabled remote-access data collection that was critical during the early stages of the COVID-19 pandemic. Data collected at the Structural Biology Center at the Advanced Photon Source has resulted in more Protein Data Bank deposits than any other facility.

Notably, BER's enabling infrastructure facilities are most often recognized as world-leading when they thoughtfully combine technical capabilities, community-tailored data analytics, and active community building. Virtual resources such as the DOE Systems Biology Knowledgebase (KBase) also help to nucleate research communities by providing a toolkit of software applicable to microbial systems biology. All of these world-leading facilities face international competition and will require targeted support to maintain their leadership positions.

6.3.1 Need for Integrated, Long-Term Infrastructure Planning

BER's enabling infrastructure capabilities currently operate as an independent collection of DOE user facilities and project-based services. There is some collaboration among biological systems science resources, such as JGI, EMSL, and structural biology and imaging capabilities at BES light and neutron facilities on an operational basis. However, long-term strategic oversight across the entire portfolio of capabilities appears to be lacking. A long-term (5- to 10-year) roadmap for BER resource development is needed that considers the capacity requirements of the research community and drives development of a unique or transformational capability. Such a roadmap would provide BER users with a significant competitive advantage internationally.

There appears to be no strategic joint planning activities with other DOE offices or agencies to identify opportunities for collaborative or synergistic infrastructure development. As a result, BER's enabling infrastructure is quite uneven in its capacity, quality, and support models. There are world-leading capabilities, such as JGI and ARM, but their leadership positions are under threat by strategic facility developments worldwide, where such integrated, long-term planning models exist. Generally, BER facilities and services are independently operated, and integration, needed by users to support complex scientific goals, is an afterthought that has barely made progress over the past decade. The recent NVBL effort demonstrated the usefulness of an integrated set of capabilities ranging from computing and data to leading experimental facilities (see Case Study: The National Virtual Biotechnology Laboratory—DOE's R&D Response to COVID-19, p. 95). However, NVBL also highlighted the enormous human effort needed today to execute a project that uses such a diverse set of enabling infrastructure capabilities.

The recent launch of the Office of Science Integrated Research Infrastructure Architecture Blueprint Activity represents a DOE-wide first step in this direction that is highly welcome. Furthermore, ARM, EMSL, and JGI leaders were key participants in the 2020 Office of Science user facilities roundtable on COVID impacts (U.S. DOE 2021b), which focused on cross-facility conversations for sharing observations, challenges, opportunities, best practices, and lessons learned. A direct outcome from this roundtable was the recognition of the value in such recurring cross-facility meetings and discussions. In December 2022, the 28 Office of Science facility directors will meet with Office of Science leadership and discuss issues that affect all user facilities. At this meeting, topics will

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CASE STUDY

The National Virtual Biotechnology Laboratory—DOE's R&D Response to COVID-19

science.osti.gov/nvbl

With funding from the CARES Act, DOE's Office of Science established the National Virtual Biotechnology Laboratory (NVBL) in March 2020 to combat the COVID-19 pandemic. NVBL brought together the broad scientific expertise and resources of DOE's 17 national laboratories to address medical supply shortages, discover potential therapeutics, develop and verify COVID-19 testing methods, model disease spread and impact across the nation, and understand virus transport in buildings and the environment. DOE had never assembled a research team of this scale, despite its history of rallying resources to support other national and international crises, such as the Deepwater Horizon oil spill (2010), Fukushima Daiichi nuclear disaster (2011), Aliso Canyon natural gas leak (2015), Ebola outbreaks (2014 to 2015), and Hurricanes Katrina (2005) and Sandy (2012).

Notably, NVBL research was successfully conducted in only 8 months, with no lead time for start-up preparations. Playing a critical role in this work was DOE's enabling infrastructure, including world-class user facilities such as light and neutron sources, nanoscale science research centers, sequencing and biocharacterization facilities, and high-performance computing facilities. The collaboration of experimental and computational user facilities was key to NVBL achievements, which are outlined in a recent report (U.S. DOE 2022a). Here, the focus is on NVBL research in molecular design of COVID-19 therapeutics to illustrate the value of an enabling infrastructure integrated across diverse capabilities.

Molecular Design of COVID-19 Therapeutics

At the pandemic's onset, there were no approved therapeutic options beyond treating COVID-19 symptoms. In the months since, only a few medicines have received U.S. Food and Drug Administration emergency use authorization for directly treating COVID-19. To accelerate discovery of small molecules and antibodies that interact with key viral targets, NVBL assembled a Molecular Design team that leveraged DOE national laboratory capabilities and analytical resources in high-performance computing, artificial intelligence (AI), structural biology, and chemistry. The multidisciplinary team focused on identifying small molecules and antibodies that inhibit all life cycle stages of the virus responsible for the COVID-19 pandemic: severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This work capitalized on an integrated computational and experimental platform established at the national laboratories.

The design platform's starting point included structures of viral proteins, multiple antibody templates developed for earlier coronaviruses, and databases of the chemical structures of small molecules for experimental confirmation (see figure, p. 96). These inputs were fed into a computational approach that combined simulation and machine-learning methods, along with structure- and sequence-driven models, to iteratively design, make, and test new molecules. Data from experimental assays and structural characterization were then fed back into the computational methods for multiple rounds of design. Platform outputs included small molecules and antibodies with confirmed inhibition of a viral protein and predicted probability for good physical and safety parameters. All project data will be made public, and team members are partnering with public and private organizations to further advance these discoveries along the pathway to clinical impact.

Takeaway

An enabling infrastructure coupled with diverse capabilities can be leveraged for a rapid, impactful response to national needs or emergencies.

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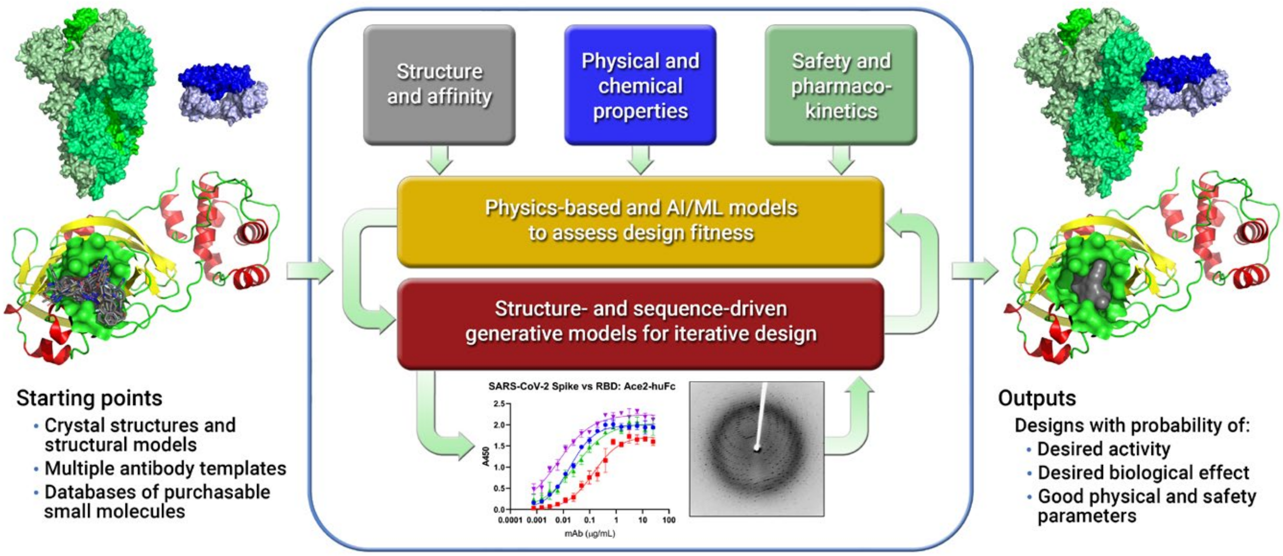
CASE STUDY



Molecular Design. Integrated computational and experimental platform for designing COVID-19 therapeutics. [Courtesy Oak Ridge National Laboratory]

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Antibody Discovery

The team's design goal was to modify three existing antibody scaffolds known from prior SARS outbreaks to create new antibodies that effectively bind to and neutralize SARS-CoV-2. The team used AI methods to sample more than 10^{40} possible antibody variations, from which about 300 designed antibodies were generated and experimentally screened. Using this combined computational and experimental approach, the team identified and experimentally confirmed hits for all three antibody scaffolds. For antibody scaffold 1, the team performed two rounds of optimization and then identified an antibody experimentally confirmed to disrupt binding of the SARS-CoV-2 spike protein to the human ACE2 receptor at ~100 nM potency and neutralize cell entry of a vesicular stomatitis virus (VSV) pseudovirus. For scaffold 2, the team identified four antibodies, one of which binds to the SARS-CoV-2 spike protein at 2.5 nM potency; none, however, neutralized viral entry, so subsequent design rounds will focus on improving neutralization. For the final scaffold, the team completed an initial design round, identifying antibodies that show evidence of binding to the SARS-CoV-2 spike protein.

Inhibitors of Viral Cysteine Proteases

Two viral proteases, 3 chymotrypsin-like protease (3CLpro) and papain-like protease (PLpro) are essential for SARS-CoV-2 replication and thus are important targets for pharmaceutical drug design and discovery. Both belong to the cysteine protease family, a structural family not amenable to traditional docking-based modeling pipelines (see figure, p. 97). The team therefore needed to create an integrated, comprehensive workflow that combined docking, molecular dynamics, and quantum mechanical simulation approaches. It used this workflow to identify, design, and optimize small-molecule protease inhibitors for both 3CLpro and PLpro. The computationally designed PLpro inhibitor binds to the PLpro protein then reacts to form a chemical bond with its cysteine residue, which is vital for enzyme activity. The team sent a subset of these designed

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CASE STUDY

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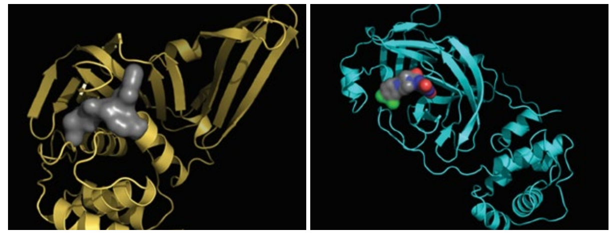
inhibitors to external research teams for screening against structurally related human proteins and for measuring the molecules' metabolic stability. The most promising covalent inhibitor is potent, selective for PLpro, and displays antiviral activity in cell-based assays, rivaling that of the RNA-dependent RNA polymerase inhibitor remdesivir in a side-by-side comparison.



Small-Molecule Design. The Molecular Design team identified two small-molecule inhibitors for the viral proteases PLpro (yellow, left) and 3CLpro (blue, right). Shown here are the PLpro inhibitor (gray, left) and 3CLpro inhibitor (multicolor, right). [Courtesy Oak Ridge National Laboratory]

DOE Capabilities Supporting the Molecular Design Team

For its iterative design cycle, the Molecular Design team used DOE enabling capabilities at (1) light and neutron facilities supported by the Basic Energy Sciences program, (2) cryogenic electron microscopy and tomography experimental facilities, and (3) supercomputing facilities supported by the Advanced Scientific Computing Research program. The team computationally screened tens of millions of small molecules against more than 100 binding sites of the SARS-CoV-2 viral proteins and docked molecules from larger databases (on the order of 50 to 100 million molecules) against a subset of the 100 binding sites. No other research organization in the world can screen as many possible targets in such a short time.

From these computational screens, the team purchased more than 2,000 small molecules for experimental validation at three DOE light sources—the National Synchrotron Light Source II, Advanced Photon Source, and Advanced Light Source—using biology-targeting beamlines that BER co-funds at these user facilities. In an antiviral screen, 56 molecules showed some inhibition of viral infection in a cell-based assay. An independent antiviral screen is now confirming the 56 hits, and researchers are conducting ongoing experiments to elucidate which parts of the viral life cycle are inhibited by each confirmed hit. The Molecular Design team's research would have been impossible without close scientific collaborations and the integration of these different facilities. Their work represents a world-leading capability that also can be applied to other large-scale molecular studies.

Continued from p. 94

focus on the integration of data and computing with the user facilities, along with remote access.

6.3.2 Impacts from Gaps in Coordinated Planning

The following are a number of additional observations identifying the impacts stemming from the lack of long-term strategic facility planning.

Long-Term Planning and Support for Project-Based Services

BER's enabling infrastructure capabilities are split into two categories: DOE user facilities and project-based services. While DOE user facilities are acknowledged to provide and require long-term stewardship and development of their capabilities in line with BER and DOE mission priorities, project-funded services have a much shorter planning horizon (3 to 5 years). This can make long-term investment and development planning difficult, which in turn limits international competitiveness. For example, the Earth System Grid Federation (ESGF) directly competes with the much more advanced services of the German Climate Computing Center (DKRZ) and World Data Center for Climate (WDCC), which has secured long-term funding and a secure facilities status. This has enabled DKRZ to be at the forefront of data service and standard developments over several decades. The United Kingdom's Center for Environmental Data Analysis (CEDA) shares a similar situation and status as DKRZ.

Another example is AmeriFlux's two-tiered support system for flux towers in the United States. AmeriFlux is open to data contributions from any flux site operator. This open policy enriches the data holdings and coverage of the AmeriFlux network. However, only 13 contracts supporting 44 flux towers enjoy long-term DOE funding. This results in a highly unstable extended network of towers. The datasets from these volunteer sites are frequently transient due to short-term funding cycles and sometimes lower in quality than the core sites. While core site support was viewed as strong and positive, the instability of this second tier of sites was viewed negatively by some international colleagues, as long-term data and stewardship are important for studies of ecosystem-climate interactions. Expansion of the number of core flux sites would advance the ability of AmeriFlux to contribute to climate science.

Access to High-Performance Computing Resources

Over the last decade, the use of computing has become ubiquitous in science, including the use of high-performance computing and data analytical capabilities to tackle the most complex scientific challenges. Yet, the number of BER users at ASCR facilities has remained the same, despite an increase in requests for access and competitiveness of proposals. This presents a significant disadvantage to the BER research community. BER has made investments in some medium-range capabilities but usually provides access only to a small set of users. In this context, it should also be mentioned that there is no clear BER policy for using cloud computing resources versus onsite capabilities.

Coordinated Exploration and Adoption of Transformational Technologies

Recent DOE reports have outlined the potential that new technologies such as artificial intelligence (AI) have in transforming scientific user facilities, from enhanced scientific discovery processes to optimized and automated operation (U.S. DOE 2020c; ASCAC 2020). BER-supported facilities have individually evaluated the benefits of novel technologies such as AI, quantum computing, and quantum sensing, but coordinated and larger-scale exploration is lacking, as is structured engagement with the AI or quantum research communities to identify challenges and potential existing or future solutions.

Disparate Data Policies

BER-serving facilities lack a common data use policy. Although different communities have disparate cultures in terms of sharing their data, there is a range of underpinning best practices that should be shared and equally implemented across BER facilities. Key issues that have not been addressed by all or have led to disagreements with their user communities include: what it means when data are publicly available (who can use it), attribution of datasets to the original creator when data are reused (either as a single dataset or in combination with others), data harvesting into third-party cloud services, varying data licenses, and long-term curation efforts needed to maintain the data's value. Generally, users find it difficult to identify and understand the numerous different data policies. Hence, better communication is needed. This situation has led to undesired consequences for early career users (e.g., being publicly shamed on social media for not understanding a particular data use policy).

Expanded Access for Underrepresented Groups

DOE does not require its facilities and projects to collect statistics related to diversity, equity, and inclusion (DEI) or request specific measures to enable underrepresented populations to gain access to its capabilities. Notably, AmeriFlux captures demographic information about its users and has a DEI strategy focused on awareness, culture, and recruiting.

Tracking Long-Term Research Impacts

BER and its enabling infrastructure capabilities are good at capturing current news stories about recent discoveries and publishing these stories in regular intervals. However, BER does not appear to track research outcomes over time to identify broadly impactful research or promote key accomplishments, such as contributions to Nobel Prizes. The availability and easy accessibility of such data is important in demonstrating a culture of world-leading science. The working group commends JGI for its new efforts in tracking the impact of its facility services far beyond the usual publication count. Other facilities should take note and consider implementing similar services. This could certainly help BER capture and present a better picture of its overall impact on science.

Data Management Funding

The Environmental System Science Data Infrastructure for a Virtual Ecosystem (ESS-DIVE) is a data repository for Earth and environmental science data. This platform enables contributors to archive and share data with supporting information in consistent formats that can be cited and tracked. Users, in turn, can efficiently find and obtain data that are easier to interpret, integrate, and analyze. ESS-DIVE does good work with the resources it has available. It is an ambitious but underfunded effort. While the combined funding for data management activities within the Earth and Environmental Systems Sciences Division (EESSD) has grown from \$3 million to \$8 million per year over the past decade, this seems insufficient to provide the long-term stewardship required for a FAIR data environment that encourages data reuse and supports modern computing technologies. The funding level is extremely small compared to other international data centers, such as Germany's WDCC or the United Kingdom's CEDA.

Fragmented U.S. Observational Infrastructure

Today, the U.S. Earth-ecosystem-climate observational infrastructure is somewhat fragmented across agencies and missions. In contrast, in the European community, carbon cycle observations are conducted within ICOS, which includes some functions of both AmeriFlux and NOAA's Global Monitoring Laboratory (flux and tower-based mole fraction observations). Further, the European Centre for Medium Range Weather Forecasting (ECMWF) has integrated carbon cycle simulations and the assimilation of tower- and satellite-based CO_2 observations into their routine atmospheric carbon reanalysis products, merging activities carried out in the United States by NOAA (weather and tower CO_2) and NASA (satellite CO_2 and carbon cycle reanalyses), an area of research highly relevant to, but currently largely disconnected from, DOE missions.

ARM airborne resources complement other U.S. airborne research platforms supported by the National Center for Atmospheric Research, NASA, and NOAA. U.S. airborne research resources compare favorably against international competitors and collectively are leading global research resources. However, within the United States, planning is not coordinated across these systems and agencies. As aircraft often are oversubscribed, coordination and prioritization across the agencies would be desirable to ensure high-priority observational campaigns have sufficient resources and efforts are not duplicated. International airborne facilities appear even more fragmented.

6.4 Future Opportunities

Future opportunities to strengthen and advance BER enabling capabilities fall into three general categories: (1) crosscutting suggestions encompassing the entire capabilities portfolio, (2) suggestions for specific existing facilities and services, and (3) opportunities for new enabling infrastructure capabilities.

6.4.1 Crosscutting Suggestions

Establish an Oversight Board that Makes Long-Term Strategic Decisions about Creating, Continuing, and Sunsetting All BER Infrastructure Capabilities

The board would develop a regularly updated strategic roadmap for future infrastructure capabilities that optimally support science areas critical to DOE missions. This roadmap should be coordinated with other relevant agencies and DOE offices to maximize investments and impacts. Examples of this type of coordination include two decadal surveys released by the National Academies of Sciences, Engineering, and Medicine in 2007 and 2017 for NASA, NOAA, and U.S. Geological Survey (USGS) research in Earth science and applications from space. Such planning efforts would enable robust community engagement and oversight by an appropriate peer board under an experienced umbrella organization dedicated to long-term planning. These types of reports also provide a documented foundation for proactive long-term planning across diverse agency investments, typically with strong community buy-in. Within DOE, the High Energy Physics program's P5 reports are comparable.

Develop an Integrated Mechanism Whereby Users Can Request Access to Multiple Capabilities at Once

Complex science challenges increasingly require access to more than one capability within BER's enabling infrastructure. BER science would greatly benefit from an integrated approach to resource requests and scheduling. A current implementation of this is the FICUS program, which includes a supporting infrastructure for seamless data exchange and integration across capabilities. More purposeful integration of AmeriFlux with other Earth system observations would be especially powerful. Potential connections could include ARM radiation and atmospheric boundary layer measurements, NEON ecosystem and flux observations, NOAA greenhouse gas and radiation monitoring, U.S. Department of Agriculture (USDA) forest inventories, USGS water chemistry data, and NASA remote-sensing measurements. Each of these programs has deep expertise and strengths but, in most cases, their observational networks do not overlap, and the use of different data standards and formats makes data synthesis and synergy across agency data collections difficult. For example, NOAA's SurfRad includes outstanding long-term radiative flux measurements at Earth's surface, but this network is entirely disconnected from AmeriFlux measurements of the turbulent water and heat fluxes needed to close the surface energy balance. Similarly, NEON sites capture extensive ancillary ecosystem data not typically available at AmeriFlux sites, and NOAA's tall-tower greenhouse gas monitoring system is largely disconnected from AmeriFlux, with the exception of the WLEF tower in Wisconsin. USDA forest inventory sites expertly document changes in forest carbon stocks over time and set the standard for these measurements and protocols but also lack integration with NEON or AmeriFlux sites that continuously measure land-atmosphere carbon fluxes. USGS monitoring of carbon transport in aquatic systems could be purposefully integrated with these other observing networks as well.

Regularly Benchmark BER's Enabling Capabilities Infrastructure Against International Resources

These routine assessments will provide important information about the capabilities' competitiveness in terms of capacity, unique resources, cost, impact, supporting prioritization, and investment decisions. Where appropriate, BER should undertake infrastructure planning to coordinate, strengthen, and optimize outcomes with similar international infrastructure.

Operate BER Data Services as User Facilities

Data services are critical to the scientific community, and DOE's new Public Reusable Research (PuRe) initiative highlights their long-term role and impact. To ensure sustained success and fitness for purpose, all BER data services should operate as user facilities with the same level of goals, oversight, and management as other DOE user facilities. This operational model would include metrics setting, collection, and reporting; stronger user representation; development of long-term roadmaps for services; compliance with international publication, citation, and repository standards and policies; informatics services; and technologies for data access. Additionally, BER should review funding for the EESSD data services, as experts and BERAC view the current level of support ($8 million per year) as low and a major weakness. European countries invest significantly more in such services. Germany, for example, spends $85 million a year on maintaining environmental data repositories and training scientists how to use them.

Establish a Cross-Organizational Team to Systematically Assess and Monitor Technological Developments and Their Potential Use for BER Science

A few times every decade, transformational technologies emerge, such as AI, quantum computing, and quantum sensing. Each of these technologies may hold tremendous potential to advance and enrich BER's enabling infrastructure. The team assembled to assess this potential should include domain experts external to the relevant facilities (e.g., enlisting ASCR researchers for AI efforts), which will lead to an accelerated and cost-effective innovation process.

Establish a Cross-Facility Working Group to Define a Foundational Data Use Policy for BER Facilities and Services

This group would also develop and share best practices in data policy, licensing, and citation.

Establish an Outreach and Training Program for Underrepresented Minorities

Because BER facilities and services are highly specialized, potential users require significant training to assess their functionalities, propose competitive research, and successfully execute experiments. University faculty and students who do not regularly access these capabilities are at a disadvantage in engaging successfully with BER's enabling infrastructure. This challenge is particularly true for organizations that support underrepresented minorities. An outreach and training program for such groups would help them learn about and successfully engage BER's infrastructure capabilities and understand how they can effectively use the resources to benefit their research.

Expand Access to Mid-Range and High-Performance Computing Resources

The current system for managing computing resource access does not provide BER scientists with sufficient capabilities. One solution might include implementing a single proposal system for all computing resources, similar to an approach used in the United Kingdom in which users are allocated resources across a portfolio of leading-edge and mid-range systems. This approach facilitates easy, efficient access to needed resources while ensuring all available resources are used to capacity. Alternatively, users from the climate community could be supported by a model like the U.S. Lattice Quantum Chromodynamics computing project (USQCD), which is funded by the High Energy Physics and Nuclear Physics programs within the DOE Office of Science. USQCD stewards mid-range computing capabilities at Fermi National Accelerator Laboratory, Brookhaven National Laboratory, and Thomas Jefferson National Accelerator Facility and manages these community capabilities to facility standards, which include clear performance metrics and regular user satisfaction reviews.

Regularly Publish Groundbreaking BER Research Accomplishments

The BER research community should consistently collect and publish an updated list of outstanding research accomplishments (e.g., Nobel Prize achievements) that acknowledges the projects and infrastructure capabilities critical to these chronicled successes.

6.4.2 Suggestions for Specific Existing Facilities and Services

Atmospheric Radiation Measurement User Facility

ARM is a world-leading facility that can be further strengthened in several areas to sustain its international standing. A challenge for ARM is limited spatial coverage, which could affect the accuracy of physical parameterizations based on data collected at its limited sites. Closer collaboration with the satellite community could help address this challenge. In fact, one expert noted that it is essential for ARM to guide the expanding international community toward establishing mechanisms for integrating climate-observing systems.

ARM is known for its high-quality data. To ensure enduring success in this area, a recent report (McComiskey 2021) identified several opportunities to further build confidence in ARM data and demonstrate that its quality and usability are comparable to other nationally and internationally supported observational programs. One suggestion was that instrument mentors are afforded time for regular recalibration and refurbishment of instruments, as well as support for refining calibration protocols for complex instruments.

AmeriFlux

Flux measurement networks provide fundamental Earth system observations, much like weather networks. Efforts to move AmeriFlux toward operating as a real-time observational network integrated with weather, radiation, and atmospheric boundary layer measurements would be powerful. Observations would be more impactful than those possible with the current mode of operation and its structure and resources. Under the current system, data availability is delayed by months for individual sites and years for network collections, and considerable effort is required to integrate network data with related Earth system observations of soils, the subsurface, atmospheric boundary layer, weather, and radiation.

AmeriFlux has DOE user facility–like capabilities and would benefit from long-term operational funding to continue its world-leading research support.

Earth System Grid Federation

ESGF has a strongly federated architecture that cannot be maintained solely by one center. To support data capacity and access, ESGF operates major data centers within DOE national laboratories, NASA, Europe, and Australia. New technical opportunities indicate that using commercial cloud providers for some ESGF services could be advantageous, simplifying management for DOE scientists and streamlining the user experience for the international climate community. Through DOE's leadership in the United States, these opportunities should be explored and funded when there is a cost benefit for doing so.

6.4.3 New Enabling Infrastructure Opportunities

Data-Centric Computing Capabilities

Researchers across the BER community—in both the Biological Systems Science Division and the Earth and Environmental Systems Sciences Division—are producing increasing volumes of observational, computational, and experimental data in the terabyte to petabyte range. Effectively harnessing the data for process studies, improved process representations, and AI training requires a new generation of data-centric computing facilities that combine large-scale, fast data storage with petaflop-level computing.

These centers also should make data accessible to scientists for processing and analysis for prolonged time periods, benefitting both specific projects and broader communities. Linking data and computing capabilities within these centers will make the resources more readily available to historically black colleges and universities and minority-serving institutions that often lack the storage and computing capacity to access the large data volumes needed for leading-edge, complex research.

Aerosol and Cloud Chamber User Facility

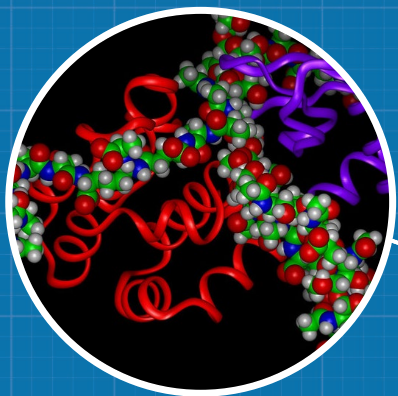
Although BER has strong atmospheric measurement and modeling capabilities, it lacks a state-of-the-art chamber to support aerosol and cloud studies. Experts suggested that an aerosol and cloud chamber user facility would help reduce uncertainties in climate model parameterizations. Such chambers are playing a leading role internationally in advancing understanding of aerosol and cloud microphysical processes.

Biosafety Level 3 Facilities

A major gap in DOE's enabling infrastructure is the lack of biosafety level 3 imaging capabilities, a need identified during NVBL research to combat COVID-19 and in subsequent discussions on future U.S. biopreparedness and response. During the pandemic, the United States relied on other countries and results from prior disease outbreaks to obtain the fundamental information required to launch research in response to the virus. In future events, these challenges could lead to delays endangering national security.

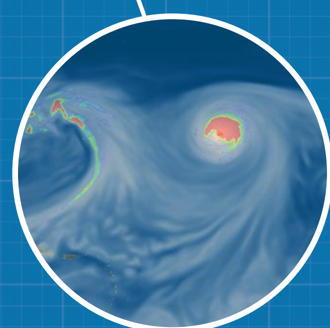
Modernization of Laboratory-Based Research Infrastructure

BER is uniquely positioned to revolutionize post-genomic research that can capture and explain biological complexity and to develop approaches and technologies reducing bottlenecks in data generation, analysis, interpretation, and translation. Toward such goals, efforts to upgrade field, greenhouse, and laboratory infrastructure would modernize data collection, support training across disciplines, and re-energize complementary biochemistry-based approaches for discovery-based research and ground-truth experimentation.



CHAPTER 7

Integrative Science



Working Group Co-Leads

John Weyant, *Stanford University*

Ann M. Fridlind, *NASA Goddard Institute for Space Studies*

Working Group Members

Allison A. Campbell, *Pacific Northwest National Laboratory (retired)*

Jennifer Pett-Ridge, *Lawrence Livermore National Laboratory*

G. Philip Robertson, *Michigan State University*

Gary Stacey, *University of Missouri*

Detlef van Vuuren, *Utrecht University and PBL Netherlands Environmental Assessment Agency*

Chapter 7
Key Findings and Recommendations

Key Findings

KF7.1 BER leads internationally in integrating climate observations and modeling, and its Atmospheric Radiation Measurement (ARM) user facility and Atmospheric System Research (ASR) program are international leaders of integrative science involving short-term field campaigns.

KF7.2 Sustaining leadership in the integration of the ARM, ASR, and Earth system modeling programs requires both maintenance of cutting-edge observational capabilities and continued access to adequate computational resources.

KF7.3 Additional leadership gains would be achieved by improving integration across the Energy Exascale Earth System Model (E3SM), the Program for Climate Model Diagnosis and Intercomparison, research in Regional and Global Model Analysis, ARM, and MultiSector Dynamics modeling efforts.

KF7.4 The DOE Bioenergy Research Centers (BRCs) exemplify interdisciplinary research ranging from detailed molecular analysis to ecosystem modeling.

KF7.5 DOE's Environmental Molecular Sciences Laboratory (EMSL), Joint Genome Institute (JGI), and light source user facilities, along with their numerous collaborators, are international leaders in integrating omics research, molecular and structural analysis, and systems biology.

KF7.6 BER is a leader in systems-level understanding such as the linkages between plant microbiomes and ecosystem function.

KF7.7 EMSL successfully integrates atmospheric science and physical chemistry with potential expansion into biological aerosols.

KF7.8 Citation analysis demonstrates integration success: BER-sponsored papers are 1.5 times more likely than non-BER papers to span two BER science areas and 3 times more likely to span three.

KF7.9 BER research could be further integrated by developing opportunities embodied in crosscutting user facility programs such as the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) project and the Facilities Integrating Collaborations for User Science (FICUS) initiative.

KF7.10 Integrating efforts across U.S. agencies is a formidable challenge leaving unrealized opportunities for further integration across BER's portfolio.

Recommendations

R7.1 Improve BER's capacity for integrative research within and beyond its research portfolio.

- **a.** Solicit support from the National Academies of Sciences, Engineering, and Medicine for synthesizing capabilities, needs, and opportunities across BER-relevant user facilities and field sites funded by DOE and other U.S. agencies to accelerate groundbreaking integrative research.
- **b.** Create sustained funding opportunities across BER, DOE, and other agencies (where possible) to advance a more integrated understanding of biological and environmental systems at multiple scales.
- **c.** Strengthen workforce capacity for integration by better supporting integrative research with targeted funding opportunities, particularly among early career researchers.

R7.2 Advance a more complete understanding of coupled human-natural systems in BER science areas.

- **a.** Include coupled human-natural system dynamics in BER funding opportunities.
- **b.** Launch a multiagency research program to improve integration across both the MultiSector Dynamics and Earth and Environmental Systems Modeling programs.
- **c.** Establish research sites for integrated long-term studies that span genomes to landscapes and the subsurface to atmosphere.

R7.3 Build international collaborations to strengthen BER's global leadership in the genomic, environmental, and climate modeling sciences.

- **a.** Work jointly with other U.S. agencies to develop an internationally coordinated effort that will provide public and private stakeholders with urgently needed climate and environmental data.
- **b.** Explore the potential for coordinating and promoting international collaborations that would leverage BER's investments in the genomic and environmental sciences, including the BRCs.

R7.4 Support integration through existing and new user facilities.

- **a.** Establish a computational synthesis center to support the pursuit of questions that demand targeted integration across disciplines and scales.
- **b.** Dedicate a cross-facilities operational budget to fund integrative science projects spanning multiple BER user facilities.

7 Integrative Science

7.1 Overview of Innovation in BER Research Integration

A key part of DOE's mission is addressing energy and environmental problems through transformative science and technology, which includes discovering and developing new energy systems and understanding and predicting their consequences at local to global scales. Enabling these advances are the fundamental scientific discoveries and tools delivered by the Office of Science. Implicit in DOE's mission is the need to understand the complex, multiscale interactions between energy systems and the environment. Attaining this knowledge requires an integrated research portfolio that promotes understanding and discovery across different subsystems of the overall energy system and enables sustainable prosperity through a vibrant bioeconomy.

As detailed in previous chapters, 45 years of BER science has helped reveal the importance of integration across different disciplines, modes of analysis, and spatial and temporal scales. Valued parts of this understanding derive from coordination with complementary research performed by other DOE programs, U.S. science agencies, the private sector, and strategically chosen international partners. The need for integrated approaches to meet energy and environmental challenges has become especially apparent internationally, with the expansion of coordinated research programs in the European Union (EU), China, Australia, and elsewhere. Many Americans today can recall DOE's origin as an executive branch agency. Enabling the full fruition of future BER research now requires a fundamental widening of perspective, scoping out from a focus on delivering long-term advances within well-delineated mission areas to a comprehensively broader strategy that actively and simultaneously stimulates scientific integration—across BER, U.S. agencies, and in collaboration with international and private-sector partners.

Individual system components reside in a network of subsystems interlinked to comprise larger systems, each with emergent properties difficult to characterize without a fundamental understanding of how components interact across subsystem interfaces. The ability to understand, predict, and ultimately manage the outcomes of these interactions depends crucially on integration—research that reveals the ways that subsystems interact to produce different outcomes. A foundational premise of systems science is that the whole is greater than the sum of the parts, which often are not additive. Therefore, understanding the whole requires integrative research.

This chapter begins by discussing the realization of and further potential for integration across BER's research portfolio. BER integration leadership is then examined using citation analyses, three examples of BER success, and one example of a lost opportunity. Then, three areas are highlighted in which global competition challenges current BER leadership in integrative science. The chapter concludes with recommendations for strengthening BER's leadership into the future. Discussions throughout draw on evidence gathered from citation analyses and multiple interviews with leading national and international experts.

7.2 BER Leadership

7.2.1 Citation Analysis Results

A topical analysis of more than 150,000 publications that were identified independently in Chapters 2–5 (to assess leadership in four BER science areas) indicates that BER is no stranger to integration. Among these publications, BER-supported articles are 1.5 times more likely than non-BER articles to contribute to two of the four science areas and 3 times more likely than non-BER articles to contribute to three of the four science areas (see Fig. 7.1, p. 106). In total, over 18% of BER-supported publications spanned at least two science areas.

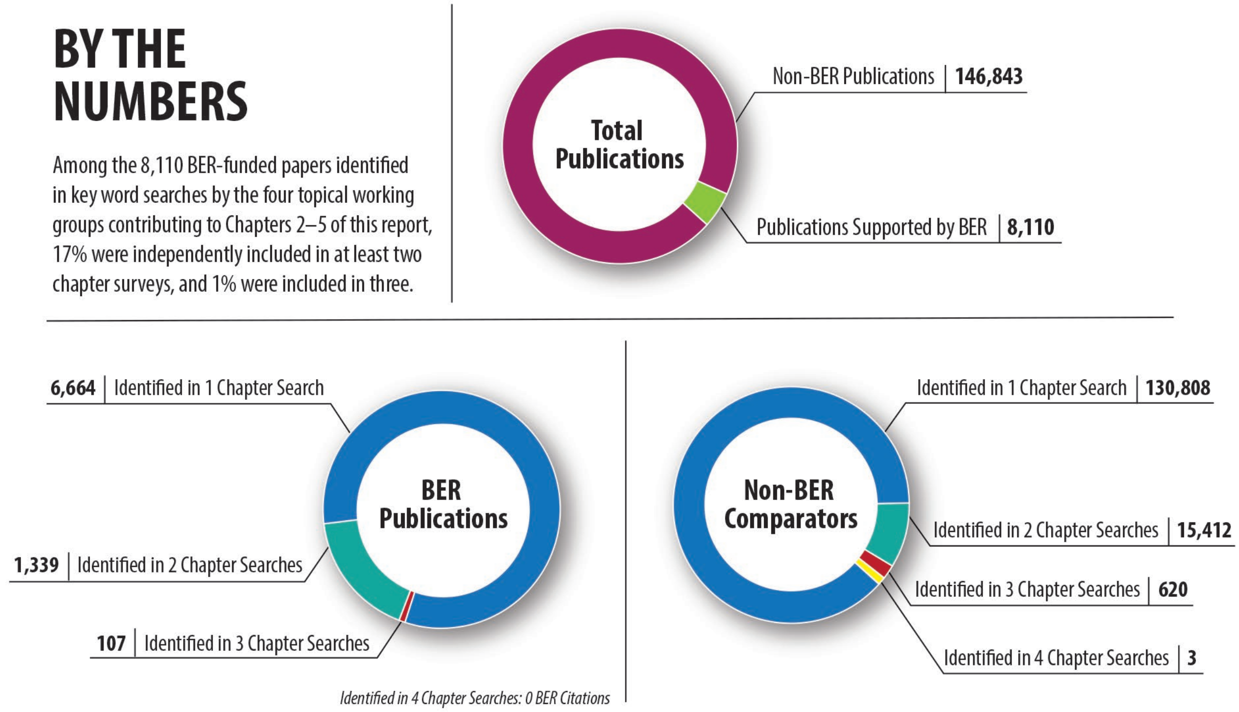


Fig. 7.1. BER Publications Cross Multiple BER Research Areas More Frequently than Non-BER Publications. A review of all BER and non-BER publications analyzed for this report (four separate topical areas for Chapters 2–5) indicates that BER publications are more likely to span two to three areas than non-BER counterparts.

7.2.2 BER Exemplars

This section highlights three successful examples of BER leadership in cross-disciplinary integration: (1) the Bioenergy Research Centers (BRCs), (2) grand challenge research efforts in biogeochemistry and membrane biology at the Environmental Molecular Sciences Laboratory (EMSL), and (3) the climate modeling and MultiSector Dynamics programs. Also featured is a counterexample from the Facilities Integrating Collaborations for User Science (FICUS) program that demonstrates the need for further effort. Examples are drawn from interviews with leading researchers who provided opinions about the current integration status across BER's portfolio and ideas for promoting further integration, including international efforts. Interviewees were chosen among thought leaders across a geographically diverse pool that spans the breadth of BER's research portfolio and institutions, including both university- and national laboratory–based individuals at multiple career stages and with broad knowledge of international programs.

Success Story 1: Integrated Research in Bioenergy—the BRCs

Bioenergy research—as pursued by BER—is inherently integrative, providing foundational knowledge to sustainably produce, deconstruct, and convert plant biomass to a range of fuels, chemicals, and other bioproducts that are otherwise produced from fossil fuels. The bioenergy pipeline stretches from field to product and thus requires expertise from plant, microbial, chemical engineering, and environmental sciences and spans scales from the molecular to landscape.

Ultimately, this knowledge must be integrated to supply industry with the fundamental science underlying effective biomass crops; agronomic practices; and biomass processing, deconstruction, conversion, and separation technologies. Together, this knowledge delivers economically viable alternatives to current fossil fuel–based products that in turn provide valuable climate and economic benefits.

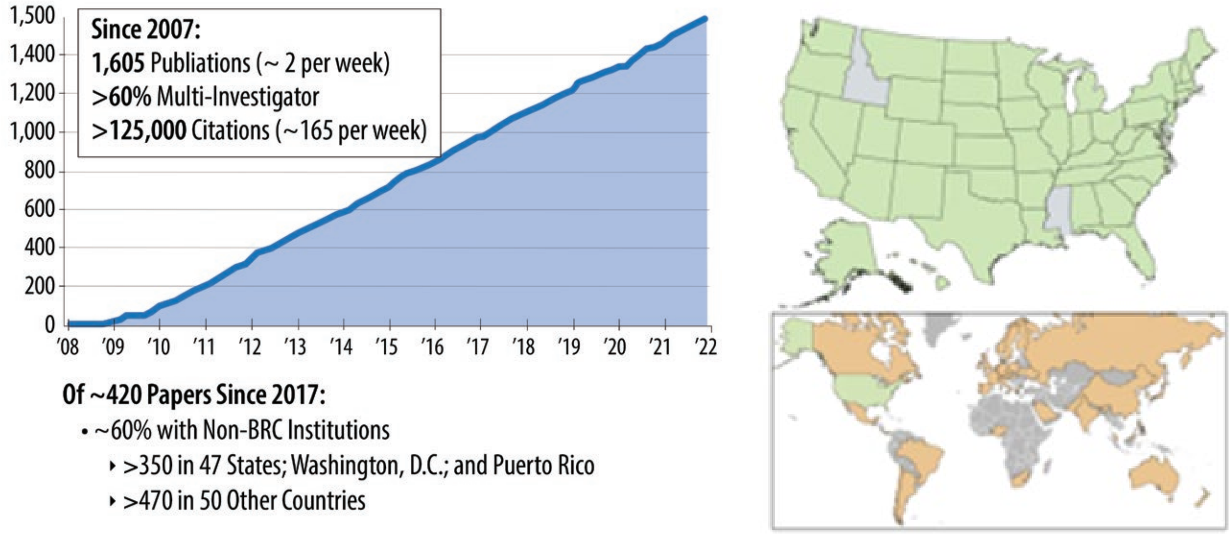


Fig. 7.2 Snapshot of Collaborative Efforts Within the Great Lakes Bioenergy Research Center. GLBRC exemplifies the collaborative reach of DOE's Bioenergy Research Centers, as demonstrated by the center's publications. More than 60% of GLBRC papers since 2017 involve collaborations with multiple coauthors from non-BRC institutions across the country (green) and world (orange). [Courtesy GLBRC]

Interviewees agreed that BER's BRC program exemplifies the integration needed to advance a future bioeconomy. The BRCs have collectively excelled in driving multidisciplinary, multi-institutional collaborations on common science problems that are often difficult to arrange on an *ad hoc* basis among independently funded principal investigators (PIs). Underpinning these qualitative assessments are BRC publication metrics showing a high proportion of collaborative papers that cross laboratory and institutional bounds, both U.S. and international. For example, more than 60% of publications from the Great Lakes Bioenergy Research Center (GLBRC) are coauthored by multiple PIs from different laboratories; a similarly high proportion of these papers include coauthors from geographically dispersed non-BRC institutions (see Fig. 7.2, this page). The scientific value of such collaborations is underscored by the tendency of these multi-investigator papers to appear in journals with higher impact factors (see Case Study: DOE Bioenergy Research Centers, p. 16).

Success Story 2: User Facilities as Integrative Research Hubs

BER funds three unique user facilities integral to advancing its research objectives: the DOE Joint Genome Institute (JGI), Atmospheric Radiation Measurement (ARM) user facility, and EMSL (see Ch. 6: Enabling Infrastructure, p. 83). BER recognizes the value of these facilities as scientific hubs that can unite facility expertise and capabilities with teams of scientists from across the nation to tackle some of the program's biggest research challenges. For example, in the early 2000s, BER formally launched two grand challenge research efforts at EMSL—one in biogeochemistry and the other in membrane biology—to foster innovation and discovery through large multidisciplinary teams collaborating on EMSL-anchored research. These 3- to 5-year grand challenges brought together multidisciplinary teams of scientists from more than 20 U.S. institutions to investigate significant questions in energy and the environment. The membrane biology effort (see Fig. 7.3, p. 108) focused on membrane proteins in cyanobacteria, important photosynthetic microorganisms in the world's oceans. The biogeochemistry effort probed the fundamental question of how subsurface metal-reducing bacteria interact with and transfer electrons to the mineral surfaces on which they live. By all measures, these efforts successfully demonstrated integrative team science using a BER facility as a research hub. Raymond

Fig. 7.3. Team Science Success in Tackling Grand Challenges. Integrative efforts that unite DOE user facility capabilities and the expertise of principal investigators from different laboratories and institutions have been an effective (if infrequent) strategy within BER to address key biological and environmental questions as part of multiyear research projects. An example is the membrane biology grand challenge project at the Environmental Molecular Sciences Laboratory (EMSL) in the 2000s, which assembled a multidisciplinary team of researchers, including those pictured here. [Courtesy EMSL]

Orbach, director of DOE's Office of Science from 2002 to 2009, lauded both projects' success, stating that "EMSL is already one of the Department of Energy's most successful national user facilities, so it is a fitting place to attempt such ambitious grand challenges, where we can pair large groups of our most talented scientists with our most sophisticated analytical tools to look at very specific and vexing scientific problems. We are hopeful that this approach will become a model for collaborative research at EMSL and other DOE facilities."

Success Story 3: Climate Observations, Modeling, and MultiSector Dynamics to Advance Climate Science Integration

BER has been a lead supporter of U.S. and international research to better understand the longer-term and large-scale impacts of energy use on Earth systems (and vice versa) over the past few decades (see Ch. 5: Climate Science, p. 63). A major aspect of this leadership is BER support of integrative innovations across (1) modeling, observational, and experimental information and insights; (2) disciplinary research programs; and (3) spatial and temporal scales of analysis. The ARM and Atmospheric System Research (ASR) programs' integration of ARM and other measurements to advance global climate observations and modeling is a key example of integrative science leadership (see Ch. 5 and Ch. 6).

Two ongoing, interrelated BER modeling-based programs are particularly notable for successfully integrating research and multidisciplinary information from different projects: the Energy Exascale Earth System Model (E3SM) and the MultiSector Dynamics research program. E3SM integrates advances in Earth system modeling and human systems modeling. For example, the Global Climate Analysis Model (GCAM) developed at Pacific Northwest National Laboratory (PNNL) accounts for dynamic land-use modeling coupled with evolving socioeconomic conditions to better understand the interplay between land use, water use, and the role of human-Earth interactions (see Ch. 5: Climate Science, p. 63). The MultiSector Dynamics research program supports teams of interdisciplinary researchers who are integrating models across multiple scales (global to regional) and sectors (see Fig. 7.4, p. 109). This work is examining how different stressors interact across energy, water, land, and socioeconomic sectors and how they could adapt—especially in response to plausible extreme values in external drivers (e.g., weather, sea levels, and baseline demographics) and internal conditions (e.g., power plant characteristics, irrigation infrastructure, and the locations of people and economic activities).

Opportunity to Strengthen Integration: FICUS

While several integration successes illustrate projects that have advanced BER goals, some counterexamples highlight situations where a lack of integration has led to lost opportunities. Initiated in 2014, the FICUS program inherently reflects BER's interest in integrative science. Through this program, multidisciplinary researchers can simultaneously access resources and user facilities across the DOE enterprise. These include (1) BER's JGI, EMSL, and ARM; (2) the National Energy Research Scientific Computing Center supported by DOE's Advanced Scientific Computing Research program; and (3) beamlines and instruments at the DOE light and neutron sources operated by the Basic Energy Sciences program. Awards linking

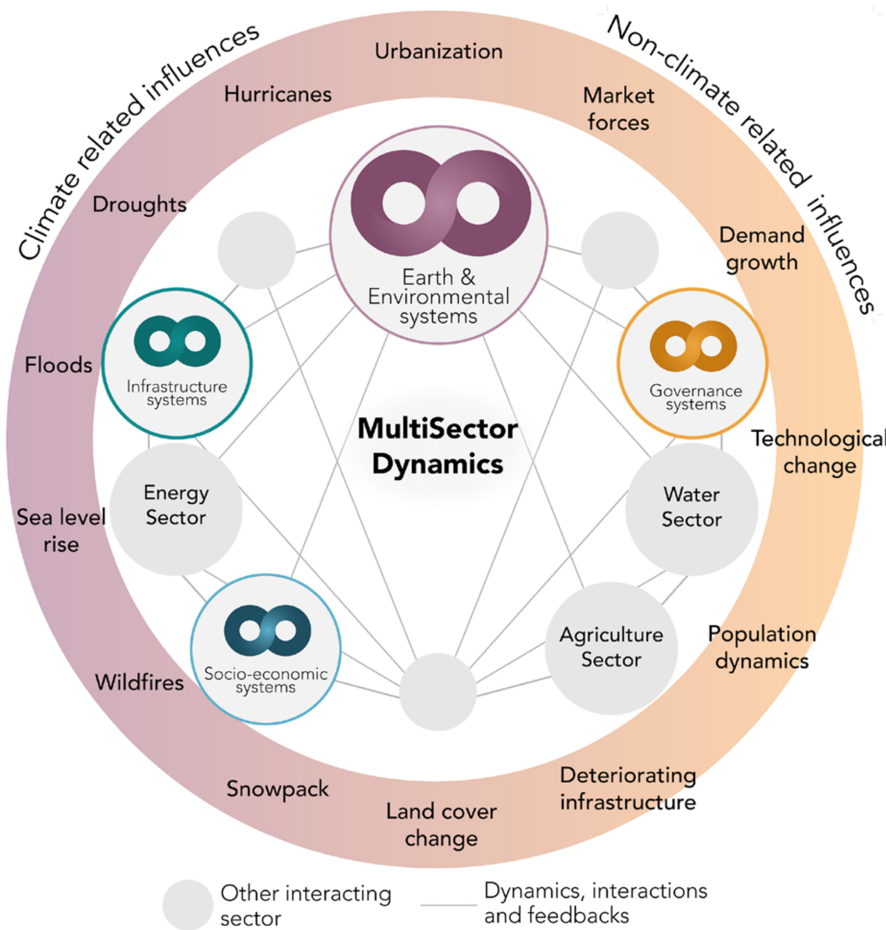


Fig. 7.4. Scope of the BER MultiSector Dynamics Research Program. Sectors are complex "systems of systems" that shape themselves through their dynamic interactions and feedback with broader Earth, environmental, infrastructure, and socioeconomic systems. [Reprinted with permission from Reed, P., et al. 2022. "MultiSector Dynamics: Scientific Challenges and a Research Vision for 2030, A Community of Practice Supported by the United States Department of Energy's Office of Science." *Zenodo*.]

EMSL and JGI's respective capacities for molecular characterization and genomic sequencing have proved the most popular category in the FICUS program. The highly competitive program supports many aspects of DOE mission research, as well as projects funded by other sponsors such as the National Science Foundation (NSF).

Because FICUS encompasses facilities from both BER's Earth and Environmental Systems Sciences Division (EESSD) and Biological Systems Science Division (BSSD), the program could serve as a key point of cross-division integration and collaboration. However, an analysis of funded FICUS projects indicates that none involved interdivisional research. Also, very few focused on flagship EESSD studies—including the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project and the Next-Generation Ecosystem Experiments (NGEEs) in the Arctic and tropics. Similarly, few FICUS projects involve national laboratory–led Science Focus Areas (SFAs), such as the Watershed Function SFA and Belowground Biogeochemistry SFA. Instead, nearly all EMSL-JGI FICUS projects are oriented toward BSSD topics, and most project PIs are associated with BSSD research awards.

BERAC conducted several interviews with BER and JGI-EMSL FICUS awardees to discuss how the program could better support cross-BER integration and scaling from molecular to ecosystem models. These researchers pointed out that ideas spanning BER mission scope do not find an easy path to funding. For example, if a study sought to use a predictive understanding of microbiomes to inform mechanisms in ecosystem models, it would likely need to de-emphasize the ecosystem modeling component to be fundable in BSSD, and vice versa in EESSD.

The separation of BSSD and EESSD research is also geographic. With the exceptions of two sites (Luquillo Experimental Forest in Puerto Rico and SPRUCE in northern Minnesota), BERAC was not able to identify sites with ongoing work funded by both divisions. In the rare instances where PIs have successfully bridged the breadth of BER mission space, the onus is on the researcher to find a way to link capabilities from different DOE user facilities and resources such as EMSL, JGI, the Advanced Light Source, the National Microbiome Data Collaborative, and the Environmental System Science Data Infrastructure for a Virtual Ecosystem. As such, the Working Group sees a ripe opportunity in the FICUS program to link more purposefully across scales; integrate empirical and modeling research; and develop protocols for archiving and associating diverse molecular, biogeochemical, and model output data streams.

7.3 Global Competition

The international scientific community recognizes the value and need for integration. In many countries, funding has flowed to large projects seeking to integrate across disciplines, geographic scales, and borders. Three efforts in particular stand out as examples of international leadership quickly gaining ground on U.S. integrative science efforts.

7.3.1 International Integrated Biology Efforts

Expert interviews pointed to several international research agencies that have developed programs that target integrated biological research; these may serve as illustrative examples for future BER programs. For example, the Research Council of Norway recently considered a Norwegian Center for Microbiome Research that focuses on how microbiomes in diverse systems (e.g., agricultural soil, the rhizosphere, domesticated animals, and engineered ecosystems) affect fluxes of methane and nitrous oxide. The Australian Research Council Centre of Excellence is evaluating a multi-institutional effort in Soil Carbon Systems, with a scope and complexity on par with a BRC. Finally, in Germany, the DFG (German Research Foundation) established so-called Priority Programmes, which provide coordinated 6-year funding for promising research topics. DFG-funded projects must be designed to promote interdisciplinary and multilocation collaboration and networking. The funding scheme includes support for researchers, including early career scientists, and instrumentation. Examples of recently funded DFG Priority Programmes relevant to BER include:

- Emergent Functions of Bacterial Multicellularity
- New Concepts in Prokaryotic Virus-Host Interactions—From Single Cells to Microbial Communities
- Systems Ecology of Soils
- Rhizosphere Spatiotemporal Organisation—A Key to Rhizosphere Functions

The rhizosphere project brings together researchers from several European countries with expertise in rhizosphere research, soil chemistry, plant genomics and physiology, soil microbiology, soil physics, exudate analysis, image and pattern analysis, and modeling. This team is identifying spatiotemporal patterns and underlying mechanisms in plant roots, nearby microbial communities, and soil minerals. They have published several outstanding articles that cross traditional disciplinary boundaries.

7.3.2 Emerging Competitors in Genomic Science

All interviewees pointed to BER's leadership in genomics as a major strength, specifically referencing JGI, which was founded in 1997 to perform sequencing work for the Human Genome Project (HGP). Since then, JGI has contributed substantially to the scientific community's understanding of plant and microbial genomes. In comparison, the Beijing Genome Institute (BGI), founded in 2003, also played an HGP role and gained early attention for its completion of the rice genome. While JGI largely limits its efforts to plants and microbes, BGI has a wider purview that includes animal and disease genomics. BGI is the largest among many strong international competitors to BER's pre-eminence in genomic science. In fact, several interviewees believe that these competitors are beginning to outpace the United States, but the group's consensus is that JGI, as a user facility, still leads globally in plant and microbial genomic science.

Beyond RNA and DNA sequencing, JGI, EMSL, and BER's structural biology and imaging resources, along with their numerous collaborators, have contributed significantly to advances in systems biology and the understanding of living systems and communities. EMSL has developed unique capabilities that greatly support the BER research community, notably a method for single-cell proteomics. Various BER-supported beamlines and resources at DOE light and neutron sources provide a strong underpinning for BER-relevant structural biology studies, enabling mechanistic insights through an understanding of structure. However, rapid advancements in genomics are quickly rendering once cutting-edge technologies routine or obsolete. Continued efforts thus are needed to ensure that the BER community retains access to innovative technologies and that BER-supported user facilities remain relevant. BSSD and user facility efforts to support synthetic biology research are laudable and offer a good example of the need to tailor research foci within the division as the science evolves. However, several experts raised doubts as to whether BER capabilities could remain cutting-edge as new innovations in genomic technologies emerge.

Because genomic technologies generate "Big Data," support for computational and informatic resources must be an integral part of the overall genomics portfolio. Although BER continues to provide strong support for these resources for microbial genomics, similar resources for plant genomics lag, despite BER's clear leadership in generating plant genomics data.

Interviewees were also in agreement that BER is an established international leader in the growing area of microbiome analysis. Indeed, the importance of the microbiome in human and animal health, plant health and performance, and environmental sustainability is increasingly coming into focus, along with a better understanding of the dynamics of microbial communities in general. Continued and expanded support for microbiome research is required to deepen these insights.

7.3.3 Europe's Destination Earth

On an international level, the European Commission's Destination Earth (DestinE) project stands out as an ambitious new program to supply member countries with interactive climate impact and mitigation strategy tools. Using the concept of digital twins, the DestinE project is integrating continuous observation, modeling, and high-performance global simulations to forecast scenarios of extreme weather events and natural disaster evolution under differing adaptation strategies. The DestinE project will be jointly executed by the European Space Agency, the European Centre for Medium-Range Weather Forecasts, and the European Organization for the Exploitation of Meteorological Satellites to meet three major milestones:

1. Deliver two digital twins focused on extreme natural events (see Fig. 7.5, p. 112) and climate change adaptation on an open-core digital platform by 2024.
2. Integrate additional twins addressing sector-specific targets (e.g., ocean) by 2027.
3. Converge twins on the shared digital platform by 2030.

DestinE will initially focus on serving public stakeholders but will later serve a larger range of users.

The DestinE initiative represents the most ambitious international effort yet undertaken to bring together high-resolution weather and climate forecasts with integrated assessment and environmental science.

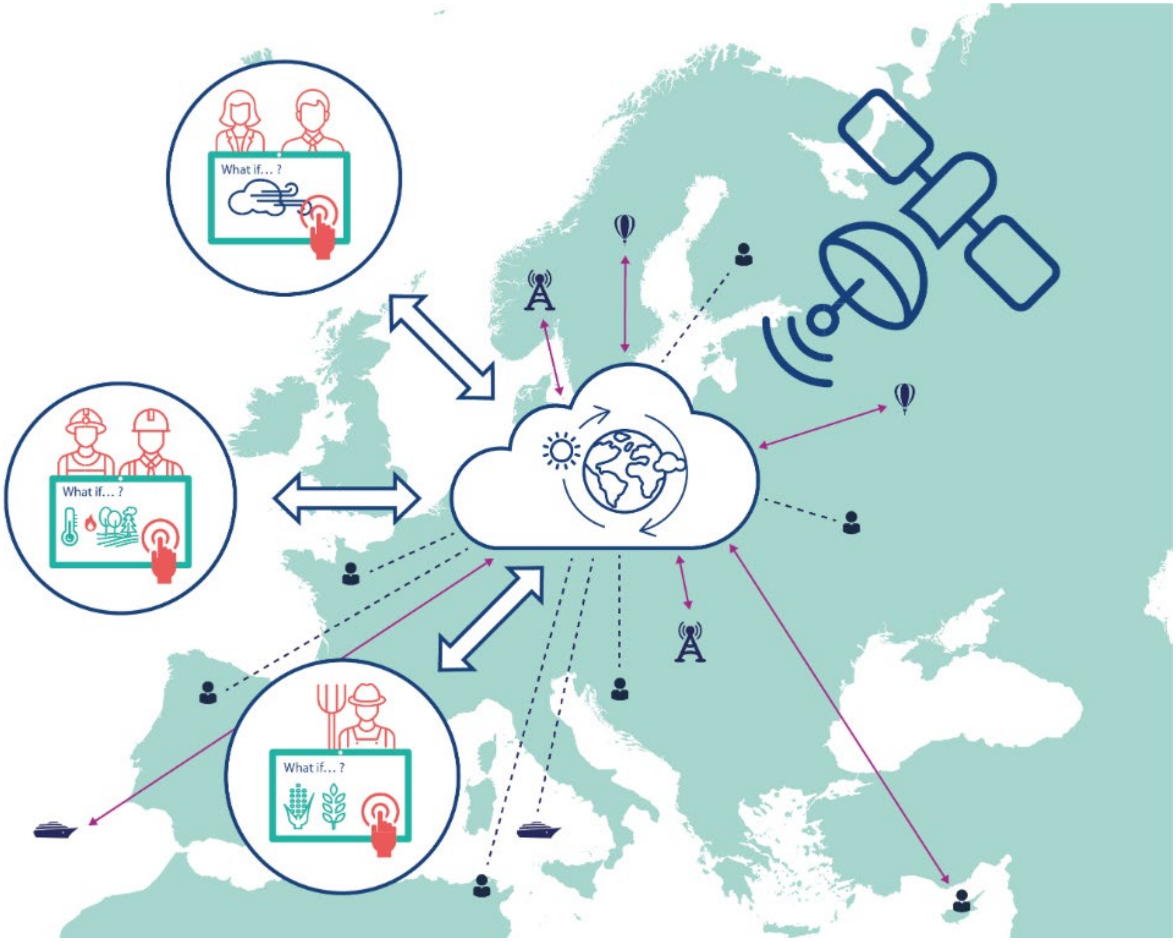


Fig. 7.5. DestinE's Extreme Natural Disasters Digital Twin. This capability will allow decision-makers to more precisely anticipate extreme natural events (e.g., flooding, droughts, and forest fires) and assess risk management strategies for civil protection, agriculture, energy, and transport. [Courtesy European Commission via a Creative Commons license, CC-BY-NC-ND-4.0]

Planning for the project began in 2019 with stakeholder meetings. These meetings highlighted the need for delivering accessible and timely operational weather, climate, and ecosystem data from a central and reliable government source and providing the precise information types needed by both public and private entities for risk-conscious decision-making. The project has selected three European global models as the initial foundation for its operational simulation framework. DestinE will deliver interactive kilometer-scale weather and near-term climate forecasts that rely on continuous data assimilation not only to obtain the most complete and accurate initial conditions but also to improve physics by studying bias correction. At this point in DestinE's development, no involvement in the Coupled Model Intercomparison Project (CMIP) is planned.

7.4 Strengthening BER Leadership in Integrative Science

This section provides 10 recommendations for strengthening BER's leadership in integrative science within and across the science domains comprising its research portfolio. Recommendations are based on an analysis of existing capacities, interviews with leading

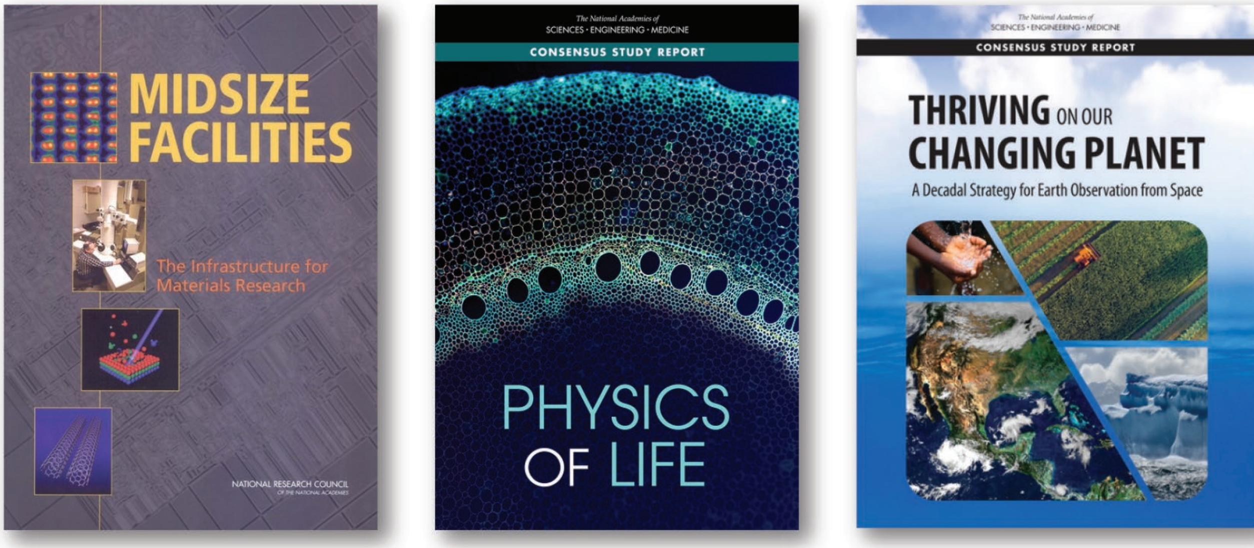


Fig. 7.6. Leadership Coordination and Community Engagement Can Accelerate Integrative Research and Maximize Investment Impact. Examples are shown of recent research reports jointly supported by other DOE offices, peer national agencies, and the National Academies of Sciences, Engineering, and Medicine. [Courtesy The National Academies Press]

scientists, and consideration of findings and recommendations in other chapters; they are grouped into four categories: (1) improving BER's capacity for integrative research, (2) incorporating human agency into the biophysical research for which BER is well known, (3) building international collaborations, and (4) supporting integration through user facilities.

7.4.1 Improving BER's Capacity for Integrative Research

Recommendation 1: Solicit support from the National Academies of Sciences, Engineering, and Medicine (NASEM) for synthesizing capabilities, needs, and opportunities across BER-relevant user facilities and field sites funded by DOE and other U.S. agencies to accelerate groundbreaking integrative research.

To maximize investment impacts, BER's strategy and roadmap for its capabilities should be explicitly coordinated with other DOE offices and peer national agencies. The foundation for such coordination and synthesis of opportunities can draw upon NASEM's successful model for interagency coordination and the use of robust community engagement to collect valuable feedback for long-term planning and coordination at the national level. NASEM reports are not binding on agencies but instead provide a documented foundation for interactive long-term planning across diverse agency investments, commonly with strong community buy-in. One example is a NASEM report jointly supported by NSF and DOE titled "Midsize Facilities: The Infrastructure for Materials Research" (National Research Council 2006; see Fig. 7.6, this page). This one-time document has a much narrower technical scope than the scope collectively represented by BER facilities, so a similar exercise for them would likely necessitate more than one report. Producing such reports would require robustly addressing critiques that suggest formalizing the long-term planning process for facility formation and evolution, as documented in BERAC's 2022 Committee of Visitors report to BSSD (BERAC COV 2022; see also Ch. 6: Enabling Infrastructure, Section 6.4 Future Opportunities, p. 99). Establishing the full breadth of facilities and capabilities to be addressed by the report process could itself provide much-needed multiagency gap-filling and facility right-sizing exercises.

BER facilities contribute to diverse research funded by multiple U.S. agencies. These wide-ranging research domains span, for example, atmospheric science—which is funded by DOE, NSF, NASA, and the National Oceanic and Atmospheric Administration—to biological physics supported by DOE, NSF, and the National Institutes of Health (NIH; NASEM 2022b). The expansive extent of these contributions motivates the need to establish an appropriately broad multiagency stewardship protocol for facilities and capabilities. Initiating multiagency horizon-scanning exercises for facility investment opportunities with National Academies support can potentially surmount long-standing barriers to integrate science areas that have historically posed formidable challenges, such as land-atmosphere interactions (see Ch. 4: Environmental System Science, p. 43).

Recommendation 2: Create sustained funding opportunities across BER, DOE, and other agencies (where possible) to advance a more integrated understanding of biological and environmental systems at multiple scales.

Prior chapters document the considerable expertise and leadership of BER science within the Biological Systems Science Division and Earth and Environmental Systems Sciences Division, ranging from fundamental systems biology to climate modeling. Of course, neither domain stands alone. Within each portfolio there are cross-cutting questions whose answers demand integrative research across and within the two divisions. Within BSSD, for example, a substantial investment in microbiome research advances an integrated understanding of plant-microbe interactions at the genomic level, with the aim of improving plant resilience to biotic and abiotic stresses. This research requires integrating environmental science at field to ecosystem scales.

Similarly, within EESSD, advancing an understanding of complex interrelations among hydrological, biogeochemical, and ecological processes requires genome-level knowledge of the microbial processes that underlie larger-scale responses. Projects like the NGEEs, SPRUCE, and several SFAs provide place-based opportunities to conduct integrative research toward understanding interrelationships within individual ecosystems and landscapes.

For more than a decade, BER has identified understanding biological systems across scales as a grand challenge. However, multiple interviewees observed that the program appears to lack a concerted effort to address this challenge head-on. There are substantial unrealized opportunities for cross-program, cross-laboratory, and cross-agency interactions. For example, several experts noted that relatively few opportunities exist for BSSD-funded scientists to meaningfully participate in EESSD-led place-based projects and, consequently, to connect genome-level organismal science with the biogeochemical and other processes that biological systems fundamentally influence. Within the NGEE program, for instance, one expert noted the difficulties that face proposals with a too-strong genomics focus (e.g., linking soil microbial community structure to biogeochemical function). Likewise, EESSD-funded scientists have few opportunities to meaningfully participate in BSSD-led bioenergy programs, despite the central importance of climate, biogeochemical, and ecological outcomes to a sustainable bioenergy future. As discussed in Ch. 2: Bioenergy and Environmental Microbiomes (see p. 11), the genome-based foundation for sustainable bioenergy development is multiscaled and complex, encompassing the functions of atoms in protein structures, the systems biology of bioenergy crops and their microbiomes, and feedstock conversion technology. However, current research does not equally address the field- and landscape-based portions of the bioenergy pipeline. They are crucial, though, for the technoeconomic and life cycle modeling that will reveal tradeoffs needed to fully evaluate the potential for transitioning energy systems from fossil fuels to sustainable bioenergy sources.

The need for integration across the BER portfolio is not limited to a single grand challenge. Targeting integrative science in each of the grand challenge areas identified in BER's divisional strategic plans and BERAC reports (BERAC 2010, 2013, 2017, 2018; U.S. DOE 2018a, 2021a) would accelerate efforts to achieve a more-integrated science understanding within and across BER mission areas. Moreover, integrative research is needed not only within BER but also between BER and other DOE programs and federal agencies. For example, BER could strengthen collaborations with DOE programs such as Energy Efficiency and Renewable Energy, Fossil Energy and Carbon Management, and Advanced Research Projects Agency–Energy (ARPA-E) and with federal agencies including the U.S. Department of Agriculture (USDA) and NOAA. This integrative approach could speed the translation of fundamental science (advanced by BER) into applied solutions. Other programs operate in different mission spaces that can complement BER research and vice versa. Thus, intentional integration holds the potential for promoting the unintentional synergies that often arise serendipitously when diverse approaches and intellects address common problems.

Recommendation 3: Strengthen workforce capacity for integration by better supporting integrative research with targeted funding opportunities, particularly among early career researchers.

A vibrant and multidisciplinary scientific community provides the foundation for BER research and must be supported and continually renewed to maintain global leadership. Early career researchers often continue to pursue science problems similar to their postdoctoral research when they start their own independent laboratories. Promoting integrated approaches to address BER grand challenges will help BER capture the research interests of this young cohort of scientists early in their careers. To accomplish this goal, BERAC recommends establishing a grant program modeled after the NIH Pathway to Independence Award (K99/R00). Such a program would specifically target postdoctoral researchers to provide support for initiating integrative BER-relevant research projects that they can continue when they establish their independent laboratories.

7.4.2 Advancing a More Complete Understanding of Coupled Human-Natural Systems in BER Science Areas

Recommendation 4: Include coupled human-natural system dynamics in BER funding opportunities.

Several experts expressed significant concern that BER is lagging behind national and international peer programs in addressing coupled human-natural systems science (see Ch. 4: Environmental System Science, p. 43). Integrating genomic and environmental findings with the human domain is crucial for effectively upscaling fundamental knowledge of biological and environmental systems to information levels that industry and society can use. The same need is equally true for building bioenergy and bioproduct components for the emerging bioeconomy and for understanding the environmental impacts and consequences of climate adaptation and mitigation options. Developing pragmatic, useable solutions requires an integrative understanding of biological and environmental systems that includes society. The current BER portfolio largely lacks this integration, except for the inclusion of economic science in BER-funded MultiSector Dynamics modeling (formerly "integrated assessment modeling"). The MultiSector Dynamics program provides a point of comparison, as well as a source of information and insights, for E3SM-level work, which the research community is now beginning to leverage.

BERAC's proposal for a "scale-aware network of energy sustainability testbeds" in the 2017 BER Grand Challenges report focuses on Earth and human trends and interactions across geographic scales and time horizons (BERAC 2017; see Fig. 7.7, p. 116). Implementing similar approaches into current BER research provides context for appreciating what the program has accomplished since 2017 and motivation for understanding why it needs to aggressively pursue this research direction even more. For example, strengthening the portfolio's human-Earth systems science component will enable the scientific community to fully understand the causes and effects of extreme events (which likely will become more severe in the years ahead) and devise ways to better anticipate and adapt to them. BER leadership would be instrumental in coordinating this effort with other U.S. agencies, the private sector, and carefully selected international partners.

The integration challenge becomes critically important in the face of rapid climate change affecting ecosystem resilience and sustainability. It is now clear that policy changes will not occur

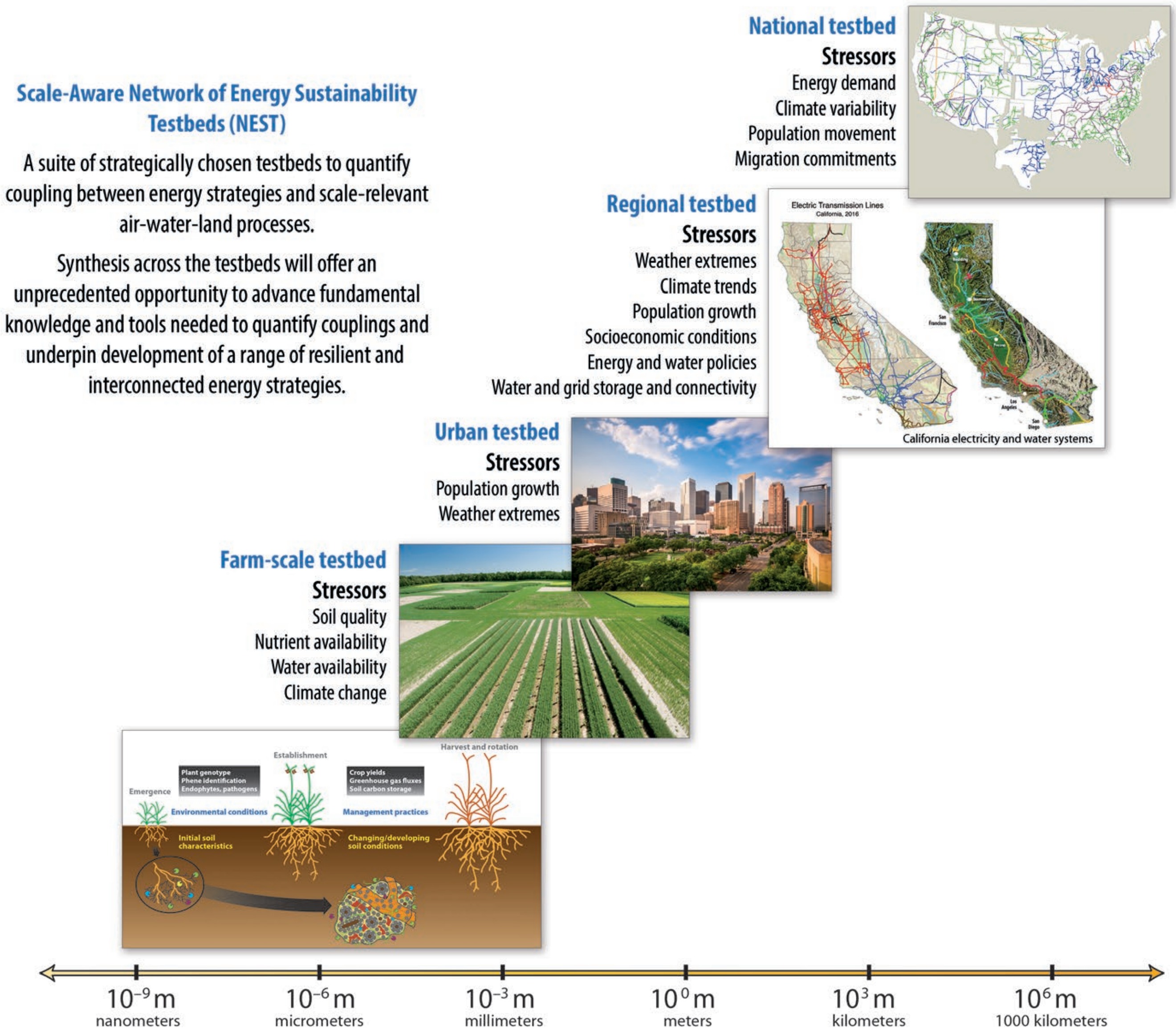


Fig. 7.7. Proposed Network of Energy Sustainability Testbeds. These testbeds comprise a suite of strategically distributed study sites chosen to span a range of scales, each relevant to a particular energy strategy and associated air-water-land forcing. Each testbed could be used for experiments, observations, and modeling to address a unique set of questions. Synthesis across the testbeds could offer an unprecedented opportunity for advancing the fundamental knowledge and tools needed to develop a range of resilient and interconnected energy strategies. [From BERAC 2017]

rapidly enough to prevent significant, negative climate impacts on ecological functions and environmental outcomes. Among other effects, these impacts threaten ongoing efforts, many led by BER, to develop a bioeconomy based on bioenergy crops. Addressing these challenges requires greater action to integrate and coordinate human-natural system science efforts. Clear opportunities exist for cross-agency collaborations, especially with agencies that have a history in fundamental coupled human-natural system dynamics (e.g., NSF) and stakeholder dynamics (e.g., USDA).

Recommendation 5: Launch a multiagency research program to improve integration across both the MultiSector Dynamics and Earth and Environmental Systems Modeling programs.

Feedback from experts indicated a consensus that much could be gained from pursuing even greater integration across climate modeling, analysis, observations, and integrated assessment. Such an approach would span E3SM, the Program for Climate Model Diagnosis and Intercomparison (PCMDI), the SFAs in the Regional and Global Model Analysis and MultiSector Dynamics programs, and ARM. For instance, interviewees suggested improving two-way communication between the climate modeling community and the integrated assessment and MultiSector Dynamics community (e.g., in the physical, behavioral, and economic dimensions of climate damages).

PNNL's GCAM team has long been a leader in integrated assessment modeling (IAM), both in the United States and internationally. However, several European teams are now established and competitive in this area thanks to sustained funding from Horizon Europe and its predecessor, the Horizon program. Historically, scientific teams at the U.S. National Center for Atmospheric Research (NCAR) and the U.K. Hadley Center have led in integrating Earth systems models and integrated assessment models. Nonetheless, BER work on ESM-IAM-MultiSector Dynamics integration challenges is likely to continue advancing the state of scientific understanding in all three communities while simultaneously identifying critical Earth and human system interactions and feedbacks that cannot be studied in isolation within each individual community. Looking ahead, one expert suggested that a program as broad as BER could explore fully coupling impact models with kilometer-scale ESMs. Since the program currently supports both types of work, such efforts could be integrated with activities in other U.S. agencies (e.g., NCAR's WRF-Hydro modeling system). Ultimately, any attempts to achieve this kind of fine-scale integration requires input from the MultiSector Dynamics community, as efforts to understand and manage individual impact sectors often involve interacting changes across many sectors and geographies.

The rest of the world has accelerated these research frontiers through innovative research programs, such as Horizon 2020, sponsored by the European Commission. Among other achievements, this program has placed the energy sector's role in Earth system evolution into an even broader context (see Fig. 7.8, p. 118). Horizon Europe also is a major funder of the Destination Earth project (see Section 7.3.3, p. 111), thus contributing to groundbreaking integration of cutting-edge, high-resolution global simulations and human-Earth system decision-making tools.

To advance its research strategy in this direction, BER should play a major role in establishing a comprehensive long-term research program in integrative human and Earth systems analysis across relevant U.S. agencies, coordinating and collaborating with the private sector and the international research community as necessary. This effort will require additional resources, but given the major societal challenges humanity faces, these resources will be invaluable to the research community and society at large.

Recommendation 6: Establish research sites for integrated long-term studies that span genomes to landscapes and the subsurface to atmosphere.

Place-based research also has the potential to create both direct and indirect opportunities for integration that can enhance understanding of human-natural system interactions. First vetted in the 2013 BER Virtual Laboratory report (BERAC 2013), the Integrated

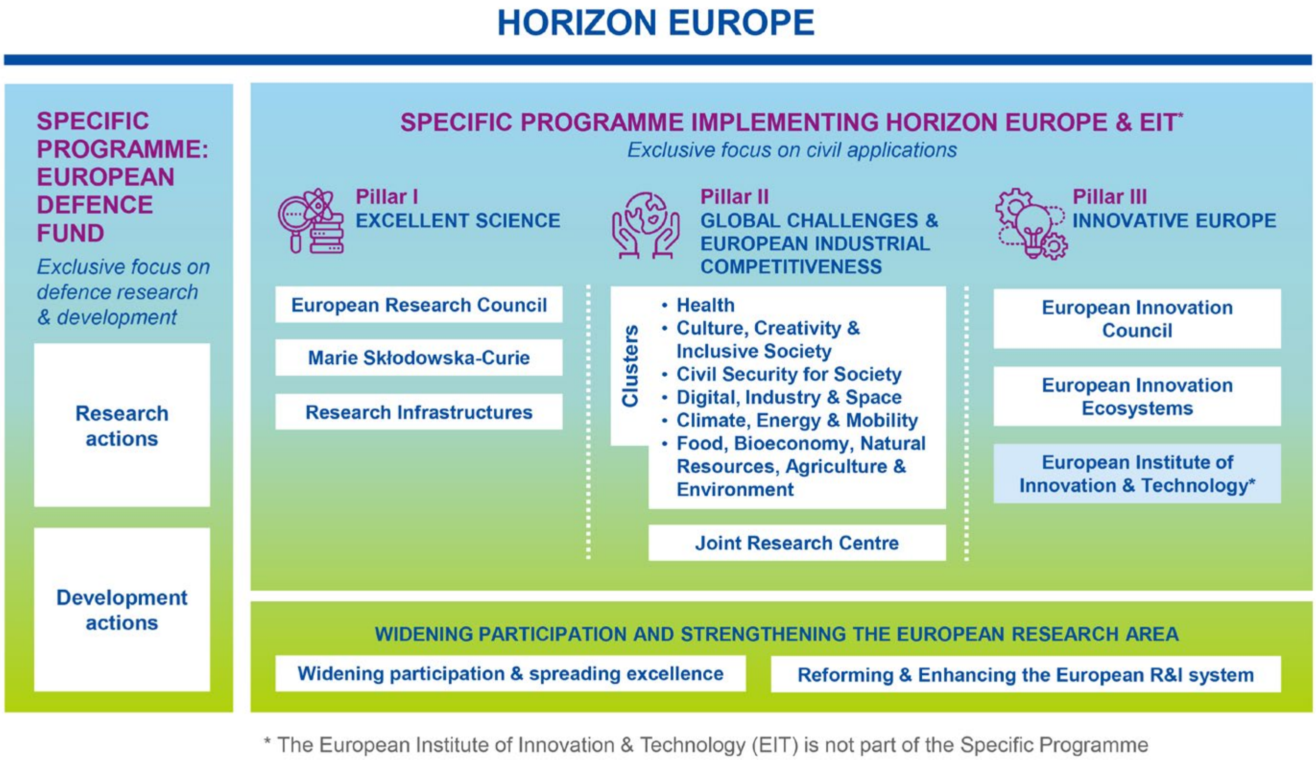


Fig 7.8. The European Commission's Horizon Europe. This program exemplifies a successful, high-level multiagency investment strategy for integrating MultiSector Dynamics and Earth system modeling. Horizon Europe's integrative strategy guides environmental policy, industrial development, and the bioeconomy through coordinated grant and infrastructure support. [Courtesy European Commission via a Creative Commons license, CC-BY-NC-ND-4.0]

Field Laboratories (IFLs) could bring together and expand laboratories in key representative ecosystems to focus on understanding and scaling fundamental biogeochemical, microbial, and plant processes that drive planetary energy, water, and biogeochemical cycles. Building on the success of earlier BER investments in study sites associated with integrated field research challenges, NGEE, AmeriFlux, and ARM programs, IFLs could explicitly engage BSSD and EESSD scientists in linking organisms and microscale processes to large-scale hydrological, biogeochemical, and climate processes.

The integrative power of conducting long-term research at single sites derives from both short-term disciplinary studies that together create a more complete understanding of site-level processes and from interdisciplinary studies intentionally designed to probe boundary-spanning relationships. Computational modeling then provides a means to test the understanding of linkages and extrapolate findings to future climates and locations elsewhere. Colocating such sites at or near long-term research sites established by other agencies could also provide some of the cross-agency integration called for in other recommendations. These agency sites include locations within the NSF National Ecological Observatory Network (NEON), NSF Long-Term Ecological Research (LTER) Network, and USDA Long-Term Agroecosystem Research (LTAR) Network (see Fig. 7.9, p. 119). BER's 2022 funding opportunity announcement (FOA) for Urban Integrated Field Laboratories (DE-FOA-0002581) is a nascent step in this direction.

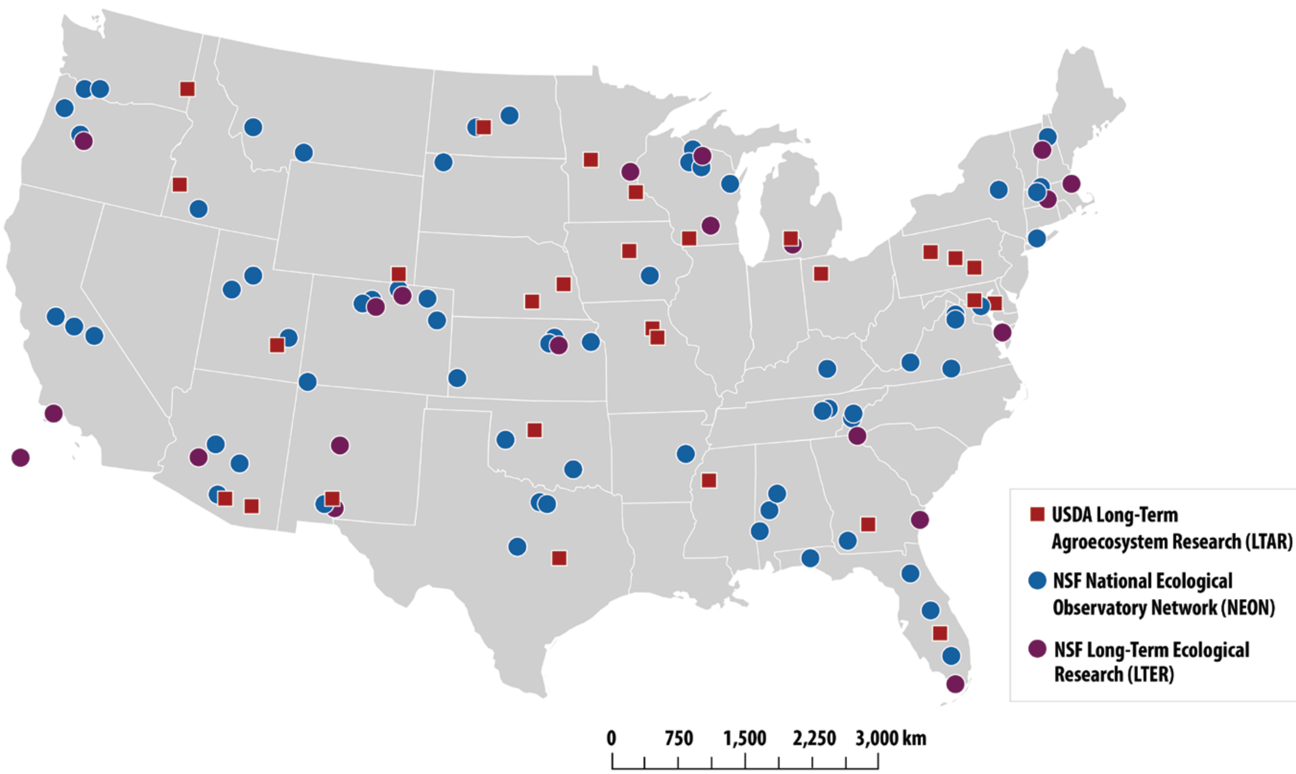


Fig. 7.9. Long-Term, Multi-Attribute Research and Observatory Networks. Distribution of conterminous U.S. sites in the National Science Foundation (NSF) National Ecological Observatory Network (NEON), NSF Long-Term Ecological Research (LTER) Network, and the U.S. Department of Agriculture (USDA) Long-Term Agroecosystem Research (LTAR) Network. DOE-supported research sites that could contribute to such networks include the AmeriFlux core sites (ameriflux.lbl.gov/sites/ameriflux-core-sites/). [Courtesy USDA]

7.4.3 Building International Collaborations to Advance Leadership in the Genomic, Environmental, and Climate Modeling Sciences

> ***Recommendation 7: Work jointly with other U.S. agencies to develop an internationally coordinated effort that will provide public and private stakeholders with urgently needed climate and environmental data.***

A U.S. multiagency-led initiative that effectively combines climate and environmental data to deliver integrative decision-making tools to public entities and industry would represent a maturation of decades of foundational science investment. Although historically useful, single-agency and sometimes duplicative U.S. efforts have not yet been effectively combined to provide the integrative science and decision support envisioned in a project such as Europe's Destination Earth. Currently, the United States seemingly has no comparable integrative strategic plan or funding allocations, but the competitive implications of trailing in this area are likely astronomical. In fact, the Financial Stability Oversight Council recently identified climate change as a potential threat to U.S. financial stability (FSOC 2021).

One expert warned that ceding the integration and interpretation of disparate climate information to private companies not only will duplicate future efforts but also risk unnecessary confusion because proprietary commercial projections are rarely open to scientific scrutiny (Fiedler et al. 2021). Yet BER cannot achieve such a degree of integration in an isolated fashion. To ensure BER's unique modeling capabilities are suited for the rapidly needed integration, BER should engage in multiagency planning as soon as possible.

> ***Recommendation 8: Explore potential for coordinating and promoting international collaborations that would leverage BER's investments in the genomic and environmental sciences, including the BRCs.***

As noted throughout this chapter, multiple international efforts aspire to advance the genomic and environmental sciences in ways related to efforts by BER. Though such efforts are almost always complementary rather than duplicative, they are rarely coordinated. A notable exception is FLUXNET, a global network of sites observing carbon, water, and energy exchange between ecosystems and the atmosphere, based originally on BER's AmeriFlux network, which is now a major collaborator. However, international collaborations for observational networks are uncommon but could yield significant synergies that might more rapidly advance BER science. BRC research, FICUS, and other BER programs might all benefit from coordination with international efforts to the extent they can be identified.

7.4.4 Supporting Integration Through Existing and New User Facilities

> ***Recommendation 9: Establish a computational synthesis center to support the pursuit of questions that demand targeted integration across disciplines and scales.***

Intentional integration can also arise by providing directed opportunities for cross-disciplinary synthesis. BER has a strong record of workshops and PI meetings that bring together scientists with diverse expertise and perspectives to assess the state of the science in a particular area and make recommendations for progress. Examples include the 2005 workshop that launched the BRCs (U.S. DOE 2006), the 2014 workshop that furthered BSSD investments in plant microbiome research (U.S. DOE 2014b), and various environmental science and climate modeling workshops leading to subsequent FOAs (science.osti.gov/ber/Community-Resources/BER-Workshop-Reports). Although invaluable for evaluating and establishing programmatic needs, these efforts also hint at the capacity for such workshops to synthesize existing cross-disciplinary knowledge in novel ways to rapidly move a field forward. BER could more aggressively pursue such integrative efforts, partly by establishing a user facility dedicated to computational analysis and synthesis, as suggested in past BER reports (BERAC 2018). Such a facility would enable targeted collaborations to synthesize and integrate disparate BER science areas while providing the visualization, computational, and training support that might not otherwise be readily available to users.

Several experts noted that the most exciting science often occurs at the interface of traditional science areas. Consequently, activities to increase such scientific "collisions" would be valuable, as would efforts to more effectively leverage the expertise of BER-supported researchers at universities, national laboratories, centers, and user facilities. Precedents for a facility aimed at these objectives exist in other domains—such as NSF's National Center for Ecological Analysis and Synthesis. Similarly, a BER facility could catalyze creative thinking that will accelerate the integration of genomics and environmental research to address questions that demand targeted integration across disciplines and scales.

Ultimately, this integrative effort would support development of the new bioeconomy and more robust ESMs. BER user facilities already have a strong track record for integration across empirical and observational domains (see Section 7.2.2, p. 106). A similar center providing advanced data visualization and computational support directed toward transdisciplinary integration could dramatically accelerate integration across BER science domains.

> ***Recommendation 10: Dedicate a cross-facilities operational budget to fund integrative science projects spanning multiple BER user facilities.***

BER user facilities are hubs of integration and could be further leveraged to enhance research that crosscuts BER programs. For example, while the FICUS program effectively facilitates and streamlines cross-facility access, it does not provide additional resources to those facilities to execute FICUS projects. As a result, the user facilities must balance budgets between FICUS projects and other user projects, thereby hampering integration efforts. Establishing a separate funding line solely for FICUS projects at the user facilities will alleviate funding pressures and lead to increased integration across BER facilities.

7.5 Conclusion

Emphasizing a more integrative BER portfolio, both internally and with external partners, is an opportunity to achieve urgently needed and comprehensive solutions to energy and environmental problems. Not capitalizing on this opportunity puts these solutions at risk. Within the Office of Science, transformative science and technology capabilities in climate change forecasting and mitigation, sustainable prosperity, and energy transitions are in danger of failing to advance critical U.S. research needs quickly enough. Moreover, all comprehensive solutions fundamentally depend on incorporating humans as drivers across systems and scales, thus requiring integration of human and natural systems science. The recommendations in this chapter are intended to enable BER to continue leading in areas in which it already excels. Perhaps more importantly, these recommendations provide opportunities to deliver the integration of transformative science and technology that is necessary for effectively translating BER science into solutions positioning the country to continue its global leadership in energy transitions and sustained industrial and economic development more generally. To be most effective, this integration is needed not only within BER but also across the myriad DOE programs and other agencies that share and amplify BER's mission.

CHAPTER 8
Strategies for People, Partnerships, and Productivity

Subcommittee Co-Chairs

Maureen McCann, *National Renewable Energy Laboratory*
Patrick Reed, *Cornell University*

Additional Contributors

Efi Foufoula-Georgiou, *University of California–Irvine*
Ann M. Fridlind, *NASA Goddard Institute for Space Studies*
Michael N. Gooseff, *University of Colorado–Boulder*
Markus Kleber, *Oregon State University*
Alistair Rogers, *Brookhaven National Laboratory*
Tim Scheibe, *Pacific Northwest National Laboratory*
Margaret S. Torn, *Lawrence Berkeley National Laboratory*
Stan Wullschleger, *Oak Ridge National Laboratory*
All working groups

Chapter 8
Key Findings and Recommendations

Experts interviewed by the mission-specific working groups and respondents to the Request For Information both provided highly consistent responses to the charge questions related to workforce, international partnerships, and the management and operations of BER's research enterprise. This chapter consolidates the entire subcommittee's Key Findings and Recommendations that emerged from these responses.

Key Findings

PEOPLE

KF8.1 BER funds academic scientists across the nation who contribute exceptional talent and new expertise to the program's mission.

KF8.2 The DOE national laboratory complex provides many positive career opportunities for BER-funded scientists.

KF8.3 Programs for undergraduates, graduate students, and postdoctoral students effectively recruit scientific talent for BER missions.

KF8.4 The lack of workforce diversity significantly limits BER's long-term leadership and the necessary growth of its scientific workforce.

KF8.5 BER frontier research successes and impacts lack visibility.

KF8.6 BER funding for high-risk discovery science and paths to independent work are rare at the national laboratories, and increased funding flexibility is desired at all career levels.

KF8.7 Real and perceived volatility in funding levels and research topics hampers workforce recruitment and retention at all career stages and impedes long-term productivity.

KF8.8 Current funding models produce high levels of professional anxiety among national laboratory programmatic staff who feel pressure to continuously secure projects that support their own salaries.

KF8.9 At some user facilities, limited opportunities exist for support staff advancement, independent research, and future career choices, leading to overwork and professional burnout. These challenges vary significantly depending on the operational model of a given facility.

KF8.10 Over the last decade, BER has seen attrition of scientific workforce talent, particularly among academic Early Career Research Program awardees, half of whom are no longer funded in the BER mission space.

KF8.11 Some BER-supported Early Career awards are limiting workforce development due to their timing and topical volatility, providing only narrow windows of opportunity in a scientist's career pathway. This impact is more pronounced for the Earth and Environmental Systems Sciences Division than the Biological Systems Science Division and its more stable approach.

PARTNERSHIPS

KF8.12 Although international collaborations are critical for strengthening BER scientific output and increasing global visibility, such partnerships are difficult for BER-funded institutions due to funding restrictions between countries.

KF8.13 BER program staff and BER-supported scientists have few resources to travel or engage internationally.

KF8.14 Meeting societal needs requires more domestic and international collaborations for ground-based observations and high-resolution Earth system modeling to improve research outcomes and ensure integration of efforts.

KF8.15 Because of its mobile facilities and ability to fund international partners, the Atmospheric Radiation Measurement (ARM) user facility excels in collaborations—both in the United States and abroad.

PRODUCTIVITY

KF8.16 BER user facilities are specially positioned to integrate researchers across BER because of their unique expertise, leadership positions, and ability to attract users.

KF8.17 The Bioenergy Research Center (BRC) program achieves strategically important BER mission goals, and its model could be applied to other relevant research areas, such as environmental microbiomes. With their integrative focus, the BRCs have excelled at building impactful and highly productive researcher networks working toward a common goal.

KF8.18 BER should maintain team-based projects combining researchers from academic institutions and DOE national laboratories.

KF8.19 Silos and mission boundaries within DOE and across agencies block the potential for science accomplishments to inform innovation and applied solutions.

KF8.20 U.S. agencies should consider opportunities to expand collaborative climate science research beyond the current facilitating role of the U.S. Global Change Research Program, which lacks allocated funding.

Recommendations

PEOPLE

R8.1 Incentivize efforts to increase workforce diversity and provide a culture of inclusivity, explicitly measuring successes and evaluating outcomes continually for further improvements using processes with broad participation.

R8.2 Invest in effectively communicating BER scientific successes and proactively convey the importance of the program's research mission to better recruit and retain top global talent.

R8.3 Support Early Career award researchers in their future and post-award career paths by providing training and opportunities for research leadership.

R8.4 Provide incentives to the national laboratories for creating and sustaining professional development opportunities for early and mid-career scientists.

R8.5 Develop and demonstrate balanced models for providing BER-supported researchers with options for both collaborative teaming paths and individual successes.

PARTNERSHIPS

R8.6 Enhance international partnerships and cross-agency cooperation by developing new funding modalities, such as joint calls with the National Science Foundation and other agencies.

R8.7 Increase opportunities for BER program managers and supported scientists to engage with their international counterparts.

R8.8 Develop new international programs and consider establishing a formal office for international activities.

R8.9 Increase fellowships, scholarships, and international exchange opportunities.

R8.10 Optimize resources and efficiencies by bridging across agencies and nations.

PRODUCTIVITY

R8.11 Promote more effectively BER's world-class programs; unique facilities; and leadership in creating synergies across observations, process studies, and system modeling.

R8.12 Secure leadership in both the science areas where BER already excels (e.g., observation and modeling integration) and in new growth areas.

R8.13 Assign facilities the responsibility of coordinating and storing the data relevant to their main area of expertise.

R8.14 Increase emphasis in modeling activities related to uncertainty quantification and uncertainty propagation for complex, multiscale systems.

R8.15 Build a productive, creative workforce by supporting interdisciplinary research opportunities for early and mid-career scientists, as is done by crosscutting organizations such as the Max Planck Institutes in Europe or Chinese institutes for environmental and climate science.

R8.16 Manage volatility, potential and realized, in funding levels and award topics.

R8.17 Use inter- and intra-agency cooperation and co-funding to foster interdisciplinary collaborations, maximize large-scale resources, and bridge Technology Readiness Levels (TRLs).

R8.18 Create a culture of communication and interaction across the TRL spectrum in DOE and among BER, businesses, and nongovernmental organizations.

R8.19 Develop integrative science opportunities as a signature area for BER.

8 Strategies for People, Partnerships, and Productivity

8.1 Inspiring Researcher Engagement with BER Missions

Multiple U.S. and international respondents defined leadership as "producing the next generation of scientists." BER could lose its international leadership irrevocably without a pipeline of the best and brightest talent to engage in the program's mission areas. Competition for this talent is international and increasingly intense between public and private institutions in rapidly emerging science and technology areas relevant to BER. The quickly evolving and highly competitive nature of ensuring next-generation scientific leadership raises important questions:

- How can BER increase its talent pool to represent the full diversity of the United States?
- How can BER best inspire and sustain academic researchers to dedicate their careers to BER science missions?
- What role can BER play to enhance desirable career tracks within the national laboratory complex for early, mid-career, and senior scientists and engineers?
- How does BER best communicate its frontier research successes to be a national and global attractor and recruiter of top prospects?

8.1.1 Increasing Workforce Diversity

BER needs new strategies to encourage underrepresented groups to pursue careers in the program's research areas. Positive first steps are the recent investments in programs such as Reaching a New Energy Science Workforce and Funding for Accelerated Inclusive Research, which seek to engage faculty and students from minority-serving institutions. However, these investments need growth and longevity. Another area of needed improvement is BER's current workforce diversity. The national laboratories now have a collection of best practices in diversity, equity, and inclusion (DEI) and many are quantitatively assessing their current support of these principles, setting goals, and designing strategies to meet them through careful allocation of resources (Gibbs and Wagner 2021; U.S. DOE 2021c; U.S. DOE 2022c, d). Evaluations are needed for funding and hiring processes to ensure that they consider and incorporate DEI best practices. Also needed are support systems to establish equal opportunities for the career progression of underrepresented minorities.

Program design, contracting, and staff training represent other opportunities to reduce barriers to engaging underrepresented groups in BER science. Respondents generally perceive the panel review process for grants as fair, and program managers are commended for their appreciation of diversity of thought and scientific experience. Suggestions for improving DEI within BER's purview include (1) setting standards for evaluating funding opportunities to reduce implicit bias, (2) requiring diversity on panels, (3) collecting data on diversity trends within BER-funded science, and (4) evaluating national laboratory hiring practices and efforts to engage underserved communities.

BER also might consider providing supplemental support to funded projects to specifically recruit and train a diverse workforce. The National Institutes of Health (NIH) and National Science Foundation (NSF) explicitly support underrepresented groups through dedicated resources to advance DEI goals, and large center-scale proposals at other agencies require balance in leadership positions and engagement with minority-serving institutions. BER could adopt similar approaches to amplify current DEI efforts.

Bureaucracy and restrictions related to establishing collaborations with international researchers for DOE projects can hinder BER leadership in both science and diversity, according to concerns raised by some interviewees and respondents to the Request For Information (RFI). One respondent stated that the requirements for bringing a foreign national into a DOE project "create a culture of mistrust" and frustrate those who are required to implement the requirements.

8.1.2 Enhancing Career Development

Support for, and the approach to, workforce development is necessarily different at national laboratories and universities. University researchers typically enjoy more academic freedom. They receive relatively short-term funding, and awards are commonly made to single investigators or small teams, which creates ample opportunities for distinguishing the intellectual leadership and contributions of individuals (especially for early career researchers). In contrast, national laboratories are funded to engage in mission-driven discovery science. They receive longer-term funding as part of large multidisciplinary teams. Although national laboratories succeed in attracting and training talented early career scientists, including postdocs and PhD students, respondents expressed concerns about the retention of theses scientists, given the limited opportunities for leadership and unique intellectual contributions on large teams (see Case Study: Can BER Influence National Laboratory Culture to Attract Great Talent?, p. 127). These same issues potentially limit DOE's ability to attract more senior scientists and diversify its workforce across all career stages. Also, many respondents noted the difficulty in disentangling the role of the DOE Office of Science from that of the national laboratories as it relates to workforce and career development.

Senior and Mid-Career Scientists

Respondents shared many perspectives on potential challenges that national laboratories face in recruiting and retaining world-leading senior scientists in BER research areas. These challenges include volatility in funding levels and priorities that restrict scientists' freedom to explore new ideas. Encouraging a less restrictive research environment with more opportunities for investigating new topics and establishing collaborations and joint appointments with universities are potential ways to simultaneously retain young scientists and attract more senior researchers. Continuity of funding and the ability to focus on scientific areas of interest are key components of research success and job satisfaction.

At user facilities in particular, staff scientists have limited time to devote to their own areas of research interest. BER might consider reducing caps on time committed to laboratory-directed research and development (LDRD) projects, providing more time for individual research at user facilities, better supporting travel to conferences, and creating more opportunities for discovery science.

According to respondents, there is a perception that DOE-funded researchers risk losing clear scientific identities and face limited career options (including work with other agencies or transitions to academia) the longer they are supported by DOE. Another perceived limitation is the lack of opportunities for independent work, partly because scientists are required to charge their time by the hour to prescribed tasks within some BER-funded projects that do not allow exploratory or collaborative research outside strictly defined areas. This practice, which is not typical in academia, is frequently referenced as overly restrictive for scientists choosing between a university or DOE national laboratory career. Although BER's very large-scale collaborative grants offer the benefits of unique, sustained, and multidisciplinary team science, mid-career researchers in these projects face challenges trying to distinguish themselves scientifically and expand their leadership roles.

Respondents suggested that single principal investigator (PI) or small-team grants could stimulate creativity and innovation while providing opportunities for mid-career scientists to distinguish themselves. They also noted that the number of such grants likely would be limited by the staffing levels of BER program

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CASE STUDY

Can BER Influence National Laboratory Culture to Attract Great Talent?

The DOE national laboratories represent one of the world's premier research infrastructures. Their greatest asset, though, is their people who are inspired by the opportunity to shepherd an energy transition, combat climate change, build sustainable prosperity, and guard nuclear security. Succeeding in these missions requires DOE and its national laboratories to be equally vested in the success of these people.

America is experiencing a post-pandemic shift in work culture. The zeitgeist is captured by Adria Horn, a military veteran, in an article from McKinsey Consulting: "The emotional ties that may have bound people together during the pandemic work period have waned, and now they will seek opportunities not only to unpin their clipped wings but to fully expand them in ways that they wouldn't have let themselves do previously." In a 6-month study in 2021, 40% of employees who left their job did not have another one lined up. McKinsey Consulting found a profound disconnect between the reasons these employees gave for leaving their jobs and the reasons their employers thought they left (De Smet et al. 2021; see figure, this page). Beyond better pay or the ability to work remotely,

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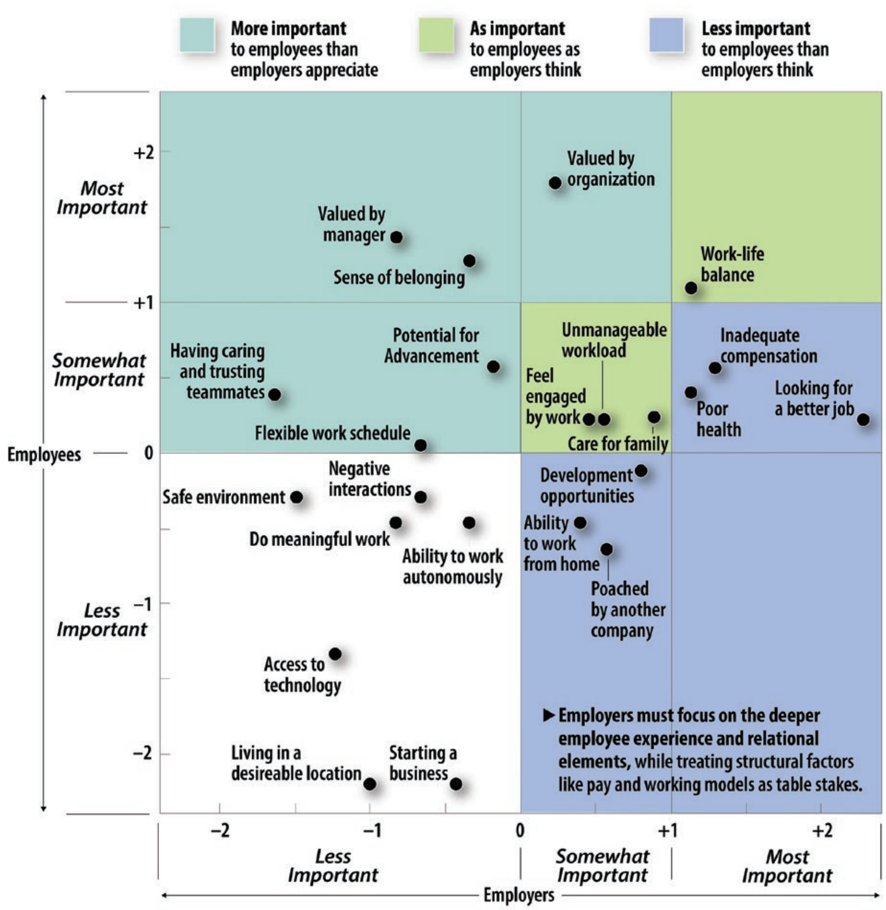

Employer and Employee Perspectives on What Matters Most. This graph highlights differences in factors that employees and employers viewed as important during a 2021 workplace study. Employers tended to overlook relational elements that were key drivers of employees leaving the workforce, such as lack of belonging or feeling valued at work. [Reprinted by permission from Exhibit 5 from "Great Attrition or Great Attraction? The Choice is Yours," September 2021, McKinsey Quarterly. www.mckinsey.com. ©2022 McKinsey & Company. All rights reserved.]

CASE STUDY

Continued from previous page

employees want to feel valued, have a sense of belonging, be part of a team that cares about them, and have a pathway to advance. The take-home message of the study is that employers that recognize and adjust to this cultural shift in the workplace will have a competitive advantage in recruiting and retaining talent.

Within the national laboratory system, some staff have opportunities for professional advancement and some feel engaged and included in laboratory objectives, according to respondents. However, management quality is inconsistent, and national laboratory staff are experiencing considerable burnout and high levels of anxiety due to the current funding model's pressure on programmatic staff to continuously find projects that support their own salaries. Similarly, respondents report that few opportunities exist for advancement or independent research at some user facilities and that facility support staff are overworked, risk professional burnout, and face limited future career choices.

There is no reason to assume that national laboratories are immune from the cultural shifts that will contribute to either great attrition or great attraction in the U.S. workplace. But what if the national laboratories were positioned to be great attractors of global talent? BER and DOE should consider how to influence the culture and climate across the national laboratory system to promote inclusivity, improve opportunities for personal and professional development, and mitigate sources of stress and anxiety.

Imagine if the best and brightest global talent could be engaged in DOE missions because national laboratories are known as destinations that value and support every employee. Imagine a future workforce that is creative, empowered, and characterized by a deep sense of community and belonging while energized to solve the grand challenges of our time. Imagine what could be achieved by driving professional development throughout the national laboratory workforce and "unpinning those clipped wings."

Takeaway

DOE and the national laboratories need to prioritize, with time and investment, workforce development.

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managers. Setting baselines for grant size would be important, with several respondents suggesting the grants minimally support 1.5 to 2 full-time equivalents.

Mid-career development strategies at other agencies or institutions might serve as useful examples of potential opportunities. Some NSF grant mechanisms allow mid-career scientists to pivot their research programs and partner with mentors to change or evolve their research focus. The Netherlands take a long-term approach to mid-career development through their Vici Talent Programme, which is similar to the Office of Science's Early Career Research Program (ECRP) but provides grants to outstanding mid-career scientists. DOE could consider a similar approach for developing more opportunities for mid-career researchers.

Workforce development is largely the responsibility of the national laboratories. However, BER can play a more active role in this process by offering an array of smaller grant opportunities across all career stages while also integrating assessments of workforce development into its major collaborative grants (e.g., the triennial reviews of Science Focus Areas).

Early Career Scientists

The ECRP is an effective way to recruit, support, and train the next generation of scientists, according to many respondents. These prestigious awards are critical investments, both scientifically and in terms of workforce development. Although respondents favorably view ECRP (with one noting that many other agencies lack comparable programs), they offered suggestions for improvement. For example, BER could (1) better advertise the program to ensure all eligible applicants know about the opportunity and (2) lengthen the time between when proposals are requested and when they are due.

BER's two divisions—the Biological Systems Science Division (BSSD) and the Earth and Environmental Systems Sciences Division (EESSD)—implement the ECRP request for proposals differently. In EESSD, ECRP topics are often very narrow and rotate among the program areas in a manner that limits consistency and continuity. EESSD is limiting its ability to capture novel and transformative ideas by overly restricting the focus of its ECRP requests for proposals, according to some respondents. As a result, early career researchers may only have one opportunity in their careers to apply for ECRP awards when their expertise, ideas, and eligibility align with the request for proposals. Another effect of BER's current ECRP approach is that proposals typically do not suggest science that crosses BER organizational boundaries.

Narrow definitions of an "early career researcher" may have unintended consequences. For example, the American Society of Plant Biologists noted, "one eligibility criterion for the ECRP award—the number of years from gaining a PhD—should be reconsidered, given the different paths today's scientists take to a faculty position (time in industry, multiple degrees, career-life balance decisions, etc.)."

BER investments in ECRP scientists do not realize their full value unless awardees have clear professional development pathways beyond their initial grants. Respondents noted the challenge for national laboratories in aligning their ECRP candidates with internal succession planning. Unlike universities, national laboratories need to find other projects that can support their Early Career award winners once their grants end. As a result, some national laboratories filter ECRP candidates, potentially limiting the range of ideas presented to BER.

Several ECRP awardees also noted difficulties in remaining in the BER community after their projects end because of a lack of funding opportunities. This challenge highlights the need to train early career scientists to write competitive proposals for the mission-driven science that BER supports. Some national laboratories already support development of proposal-writing skills, but these efforts are perhaps not as widespread as they could be.

Again, several respondents suggested that BER dedicate funds to a small-grants program that might support exploratory research beyond narrowly defined mission-oriented topics. Such grants would provide early career researchers with time to develop proposal-writing skills and experience in leading, conducting, and managing their own projects. Ideally these small grants also could serve as transitions back toward large, ongoing mission-oriented research projects. Other potential strategies for improving retention of early career scientists include:

- Recognizing researchers for their overall contribution as opposed to their impact on a single project.
- Retaining senior scientists who can collaborate with early career scientists.
- Promoting organizations and research success stories at large conferences.
- Adjusting funding mechanisms (see "Funding Cycles for Projects and User Facilities" section, this page).
- Incentivizing the development of university courses targeting the skills needed for BER-focused research.

Funding Cycles for Projects and User Facilities

The frequency and duration of BER funding cycles for projects and user facility support can pose particular challenges for both early and mid-career researchers. BER funding cycles can throw researchers' career development off track if they miss applying for an annual or even less-frequent funding opportunity or user facility call due to life events such as child or parental leave. Knowing in advance when calls for proposals will be announced would help PIs, along with establishing rolling funding opportunities that could support off-cycle ideas and enable researchers to reset their careers after life disruptions.

In addition, respondents strongly viewed 3-year, nonrenewable funding cycles as problematic. Such cycles are incompatible with the funding of graduate students, since obtaining a doctorate takes substantially longer than 3 years in the United States. In contrast, BER ECRP awards are typically 5 years, a duration enabling PIs to be more creative, innovative, and ambitious. Other potential funding durations and structures to consider include (1) 3-year grants that are renewable or explicitly intended as seed projects for downselecting and then launching larger collaborative projects or (2) 10-year grants with decisions on funding continuation in year 5. Japan has good examples of these types of structures that DOE might review and evaluate.

Training the Non-PhD Workforce

BER's impact from supporting the training of PhD students and postdoctoral researchers is significant. However, the program's national and international leadership is not solely contingent on people with doctoral degrees. Competition and demand are and will continue to be high for specialized staff who can operate facilities, manage them, and support and use cutting-edge emerging technologies, such as artificial intelligence, edge computing in cyber-physical systems, and quantum computing. An increased focus on individuals with bachelor's or master's degrees likely will be warranted, subject to specific staff roles and focus. Consequently, specialist programs, including practicum training such as those found in Germany and Japan, will be more important than doctoral-level theory. Example practicums could involve sensing, control systems, the use of feedstocks in conversion processes, and software engineering with embedded intelligence. A powerful approach to implementing these practicums might include demonstration facilities at national laboratories in partnership with community colleges and the private sector.

BER could potentially enhance workforce development in several ways. NSF and NIH both have strong programs to support workforce development, including sponsored internships for students to work in nonacademic settings. Similar opportunities for DOE laboratory personnel may enhance opportunities for innovation.

8.1.3 Developing a Communications Strategy for Workforce Recruitment

Respondents raised several issues regarding BER's communication strategies. Although many example achievements substantiate BER's scientific leadership, the scientific community generally does not associate these successes with the program. This lack of visibility, both nationally and internationally, has implications for workforce recruitment and for communicating BER's success stories to audiences including Congress, stakeholders, and the public.

BER needs to become more visible and accessible, according to several respondents representing the continuum of BER science. Academic PIs and their partners interact, experience, and perceive BER in a fundamentally different way than those within the national laboratory complex. Many researchers feel that BER-funded science is not fully open, that there is an "in crowd," and that they lack the knowledge to break into the program's mission-driven funding environment. These are major challenges to engaging underrepresented minorities and achieving diversity, equity, and inclusion within BER programs. The BERAC subcommittee identified two primary barriers to expanding BER science collaborations within the broader scientific community. Both involve a lack of understanding of (1) how non-BER scientists can receive funding and thereby contribute to DOE missions or (2) how non-BER and BER scientists can access novel DOE resources and capabilities.

Although some annual funding opportunity announcements (FOAs) specifically target the academic science community, many in that community do not fully understand how FOA priorities emerge or how best to formulate a FOA response aligned with Office of Science missions. Clear guidance is needed that describes ways to engage DOE programs, explains DOE mission-oriented culture, and outlines strategies for working with DOE scientists as potential collaborators. BER programs hold town hall events at large conferences (e.g., the American Geophysical Union's annual fall meeting), but additional guidance from and access to program managers (e.g., online office hours) would directly benefit researchers unable to attend conferences.

Another barrier scientists can face is gaining access to DOE resources, such as novel instrumentation, laboratories, and field platforms, that can advance their science—a challenge that surprisingly confronts both academic and national laboratory researchers. A research group must often write two proposals: one to conduct the proposed science and another to use unique equipment or capabilities at a DOE user facility. However, independent groups that review both proposals often conclude that neither proposal is worth supporting unless the other one is (a scientific catch-22). This challenge is compounded by different timelines and different decision-makers involved for both proposals.

Some user facilities, such as the Environmental Molecular Sciences Laboratory (EMSL), regularly reach out to the broader scientific community to explain how their administrative and technical systems work and to provide points of contact and collaboration between facility staff and potential users. Additional workshops or online presentations would prove useful from other Office of Science–funded facilities that provide tools that support BER science. Another consideration is whether facilities following a centralized model (e.g., single, large user facilities) provide equal access across the community. Some capabilities, including automation and data science, could benefit more users if they were regionally distributed across the United States.

In summary, BER needs improved communication strategies to retain its talented workforce, engage new constituencies in its mission space, and continue to attract global talent.

8.2 Opportunities for International Partnerships

The charge letter for the BERAC subcommittee's benchmarking effort outlines "international competitiveness" as a central focus, but respondents strongly cautioned against a strict adversarial framing of BER's leadership relative to international peers. As noted by the National Science Board's Vision 2030 report, BER must acknowledge that sustained leadership requires strongly engaging in ". . . a truly worldwide enterprise, with more players and opportunities from which humanity's collective knowledge is growing rapidly" (NSB 2020).

This collaborative perspective is particularly significant given BER's central role in addressing the emerging bioeconomy, climate change, and sustainable prosperity—all of which will fundamentally shape the future of the global collective commons. These issues cannot be adequately addressed by a single nation, much less a single U.S. agency. Environmental system science, climate science, and Earth system modeling exemplify the need for and importance of enhancing domestic and international collaborations to accelerate research impacts (see Fig. 8.1, p. 132). The scientific challenges associated with each research area require assembling teams with diverse expertise; leveraging national and regional field campaigns and data; and implementing enhanced, cross-agency and international funding mechanisms.

BER's Atmospheric Radiation Measurement (ARM) user facility and Atmospheric System Research (ASR) program have achieved notable successes in international and domestic partnerships. For example, ARM demonstrated significant leadership in supporting and internationally coordinating the Polarstern cruises during the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) polar expedition (see Case Study, p. 133). Experts noted that ARM and ASR are two of only a few BER programs to fund international partners, an activity they say should be maintained.

ARM's three mobile facilities represent another significant collaborative strength, enabling scientists to

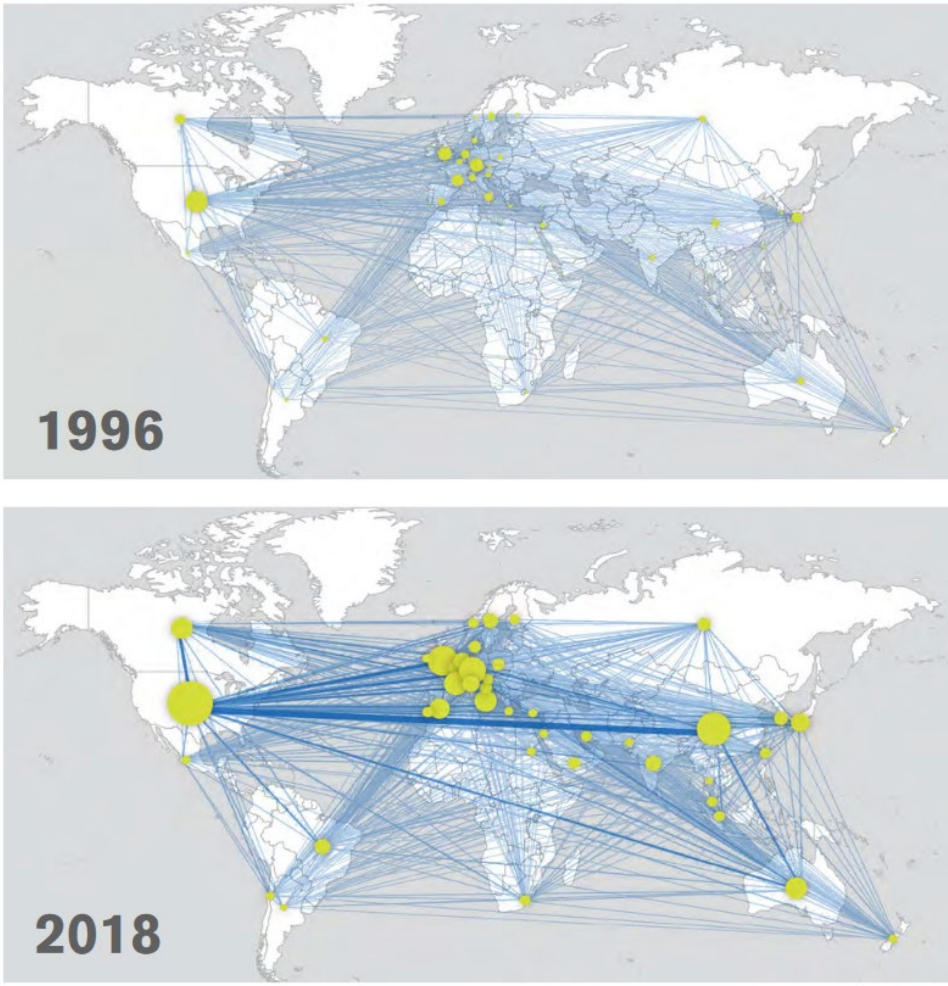

Fig. 8.1. International Collaboration Among Researchers Grows Dramatically. Collaboration among scientists and engineers around the world enhances research capacity. In 1996, U.S. researchers most frequently co-authored papers with researchers in Europe and Japan. In 2018, these connections grew, as shown by the width of the lines and the size of the circles, which denote relative number of publications. China has emerged as the single most frequent partner with the U.S. research community. [Courtesy National Science Foundation]

propose field campaigns to use these facilities to collect atmospheric and climate data from undersampled regions around the world. Proposals are open, and those submitted by consortiums have increased chances of funding. These exemplary capabilities clearly demonstrate BER's commitment to international collaboration for research observations. Domestically, the ARM Tracking Aerosol Convection Interactions Experiment (TRACER) campaign represents BER leadership through cross-agency coordination with NASA and NSF. In the climate modeling space, BER commitment to international collaboration is more difficult to discern.

BER can promote international and collaborative leadership through a variety of mechanisms. Increasing opportunities for international scientific exchange, particularly for DOE scientists, would be valuable at all career levels, stimulating new ideas and directions

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CASE STUDY

MOSAiC—Multidisciplinary Drifting Observatory for the Study of Arctic Climate

Dramatic changes in the Arctic climate system and rapid retreat of Arctic sea ice strongly affect global climate. The inability of modern climate models to reliably reproduce Arctic climate change is one of the most pressing problems in understanding and predicting global climate change.

In 2016, the International Arctic Science Committee published the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) science plan, outlining an ambitious strategy for comprehensive new observations to decisively advance coupled-system, process-level understanding of the rapidly changing central Arctic region. Spanning the atmosphere, sea ice, and ocean, as well as physical, biological, and chemical constituents, MOSAiC was conceived from the beginning as an endeavor that would demand extensive international support and collaboration. In 2014, DOE became the first U.S. agency to commit major field resources to MOSAiC, contributing an advanced Atmospheric Radiation Measurement (ARM) mobile instrument suite to the campaign's core Central Observatory. Ultimately, more than 20 countries were involved in the 389-day expedition despite the global pandemic.

In late 2019, Polarstern, a German research icebreaker vessel, set sail from Tromsø, Norway, to spend a year drifting through the Arctic Ocean while trapped in sea ice. After launch, researchers established a distributed network of diverse instrumentation on the sea ice within about 50 km of the ship, a distance similar to a typical climate model grid box. Data was gathered continuously as the sea-ice site drifted across the polar cap toward the Atlantic Ocean. Periodic, ship-based resupply missions with partner vessels provided logistical support to more than 300 experts from 16 countries onsite during the campaign (see figure, next page).

Takeaway

The Atmospheric Radiation Measurement user facility demonstrated BER's key leadership in an international partnership by operating a major component of the largest Arctic scientific expedition in history involving more than 80 research institutions from 20 countries.

Analysis of observations commenced as soon as data began to flow, opening a second phase of international collaboration. BER's Atmospheric System Research program is funding ongoing analysis of ARM observations captured during the MOSAiC expedition. This research includes characterizing central Arctic atmospheric aerosols and clouds in unprecedented detail, quantifying the radiative balance at the sea-ice surface, and linking precipitation measurements to surface snow accumulation. To analyze atmospheric particle samples collected aboard the Polarstern, scientists will use capabilities at BER's Environmental Molecular Sciences Laboratory, specifically the state-of-the-art computer-controlled scanning electron microscope with energy dispersive X-ray spectroscopy (CCSEM-EDX). A sequencing project supported by the DOE Joint Genome Institute will provide the first annually resolved microbial inventory of the central Arctic Ocean and include data on microbial biodiversity and activity across multiple Arctic climate system interfaces sampled during MOSAiC. Crosscutting analyses will enable linkage of microbial gene functions with ecosystem processes and services such as the production of climate-active gases and primary productivity. As planned, MOSAiC's observation- and laboratory-based science is already serving as an internationally supported foundation for extensive assessment and advancement of worldwide predictive modeling tools in the Arctic region.

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CASE STUDY

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BER and the MOSAiC Expedition. **(a)** The Polarstern icebreaker carried more than 50 Atmospheric Radiation Measurement (ARM) user facility instruments for the year-long MOSAiC campaign, collecting data for comprehensively studying the central Arctic's atmosphere, ice, ocean, and ecosystem. BER's Atmospheric System Research program is helping support the ongoing data analysis. **(b)** Workers load instruments, including a radar wind profiler, onto the ship ahead of its 2019 launch in Norway. **(c)** A scientist releases a weather balloon during the expedition. **(d)** Technicians work at the Met City research station where instruments were installed on the sea ice. [All images courtesy ARM]

Continued from p. 132

that would benefit BER missions. Just as diversity within scientific teams produces different approaches to conceptualizing problems and solutions, engaging different international scientific cultures would provide new research ideas and opportunities too. Academic faculty respondents noted successes in this area related to their own experiences on sabbatical leave overseas. Furthermore, BER's international reputation and ability to attract top global talent would be enhanced by bringing foreign scientists to the United States through exchanges enabling them to work closely with DOE-funded scientists. The integration of international collaborators into DOE projects for a specified duration could benefit an entire research team.

International partnerships are common in many other countries, especially the European Union. Although some DOE programs conduct research on sensitive topics not conducive to international exchanges, BER research areas are generally free of this sensitivity. As one respondent noted, "there should be no national competition in trying to understand how Earth systems and ecosystems work." Thus, opportunities for international partnerships and collaboration may be viable and provide pathways to find new common interests, even with countries that might otherwise be considered adversaries.

Notably, the Next-Generation Ecosystem Experiments (NGEE) in the tropics and Arctic are two example projects from BER's research portfolio that could significantly leverage international cooperation to benefit DOE. NGEE Tropics is largely international, with fieldwork and data collection occurring in countries such as Brazil and Panama. Similarly, NGEE Arctic, while primarily focused in Alaska, has broad opportunities for impact and collaboration across other Arctic countries. Three additional suggestions for enhancing through partnerships the scientific leadership of BER—and more broadly the Office of Science—are described below.

1. **Develop New International Funding Programs and Establish a Formal Office for International Activities.** BER leadership could institute new mechanisms for international and cross-agency collaboration. International programs that serve as useful examples include (1) a collaboration between NSF and the United Kingdom's Natural Environment Research Council; (2) the Belmont Forum, a partnership committed to advancing transdisciplinary science for mitigating and adapting to global environmental change; (3) the U.S.-Israel Binational Science Foundation; (4) several other programs managed by the NSF Office of International Science and Engineering; and (5) NSF's Accelerating Research through International Network-to-Network Collaborations (AccelNet) program, a new initiative to "tap scientific excellence around the world and provide coordinating mechanisms to support this intellectual potential for the benefit of all."
2. **Increase Fellowships, Scholarships, and International Exchange Opportunities.** More than 60% of PhD students in science and engineering are international (Burke et al. 2022), underscoring the need to increase graduate student fellowships for U.S. students to attract them to graduate studies and postdoctoral opportunities. Expanding the scientific workforce also will require providing more opportunities for international fellowships and scholarships through international exchange. With funds provided by their respective governments, several international competitors offer extensive fellowships that enable much greater mobility of graduate students across international borders. U.S. students are at a relative disadvantage for reciprocal engagement.
3. **Optimize Resources and Efficiencies Through U.S. Agency Collaborations.** BER could achieve key partnerships and develop co-funding mechanisms for larger projects with other federal agencies that support more "blue sky" research (e.g., NSF) or have complementary resources, such as computing, field campaigns, and modeling expertise. Example cross-agency programs include the Water Sustainability and Climate project and the Innovations at the Nexus of Food, Energy, and Water Systems initiative; both of these NSF and U.S. Department of Agriculture partnerships have funded significant research over the past decade.

8.3 Enhancing Research Operations, Management, and Resources

Effective communication and expanded interactions within BER; across DOE programs; and with other federal agencies, industry, and international counterparts have the potential to change scientific cultures, expand BER's recruitment of top talent, and infuse the program with new perspectives and ideas. Other opportunities to strengthen and enhance BER's research enterprise center on successfully managing funding volatility and shifts in research program continuity and priorities. Frequent horizon scanning to identify critical and needed research opportunities and challenges will also be important.

8.3.1 Leveraging Interactions Within BER, DOE, and the Private Sector

Recent DOE organizational changes reflect federal priorities to link science and innovation more explicitly. By convening Science and Energy Technology teams that cut across the Office of Science and applied technology offices, DOE has demonstrated its commitment to open lines of communication between fundamental and applied research programs. Positive steps include proposed investment in the Energy Earthshot Research Centers and single-PI or small-team awards that range from use-inspired discovery research to technology development.

Further opportunities exist for BER to strengthen communication and interactions across its divisions and with other Office of Science programs. Many respondents noted that even basic efforts to improve coordination and communication within the Office of Science are difficult due to stove-piped offices, program-specific interpretations of mission dictates, the difficultly of establishing interagency agreements, and the implied pressure to avoid program-specific taboo topics. Effective communication has the potential to change cultures across the Office of Science, ideally creating more comfort with blue sky research and with designing use-inspired experiments and approaches for a broader set of applications.

Even within BER itself, respondents noted obvious complementary capabilities across the EESSD and BSSD research portfolios, yet co-funding and other explicit support for cross-program activities are often lacking. Environmental genomics stands out as a potential example where coordination between programs might yield fruitful outcomes. Untapped potential exists for leveraging the strengths of both divisions to generate, for example, a more accurate mechanistic understanding of the carbon cycle, from microbial to continental scales.

Some BER programmatic directives, such as efforts in Biosystems Design to promote tool development for plant and microbial synthetic biology, are directly relevant to interactions with the private sector and for the emerging bioeconomy. BER-funded discovery science underpins development of intellectual property, start-ups, and new industries. For example, companies such as Gingko, Zymogen, Amyris, and Millipore-Sigma take advantage of open science competitiveness in the United States.

Capabilities in synthetic biology create economic advantage but also national security vulnerabilities. The synthetic biology community has taken steps to evaluate ethical considerations in its own research. These efforts provide an interesting model for other critical research areas, such as artificial intelligence and quantum science, and their intersections with biological and environmental research, where domain expertise becomes essential for informing scientific directions when regulatory policies are lacking. As the pace of scientific discovery continues to accelerate, BER could engage more closely with DOE policy offices to consider the balance among open science, intellectual property, limitations on commercial access to data and tools, economic competitiveness, and national security.

BER proposal solicitations are typically strategic and targeted. Although successful in many ways, does this research model need to be reframed or enlarged to secure the international competitiveness of BSSD and EESSD in the 21st century? Opening the door for transformative ideas and paradigm-challenging research is in line with DOE's mission and overall strategic goals, and it offers the potential for scientific breakthroughs and discoveries critical for addressing future environmental, economic, and energy challenges. Such a new model could strengthen ties with academia by diversifying funding mechanisms between national laboratories, academic institutions, and PIs of diverse backgrounds and career stages. Moreover, formalizing joint appointments, student exchanges, sabbaticals, and short visits could contribute to the retention of national laboratory scientists whose professional development could benefit from a dual academic-government environment.

8.3.2 Managing Funding Volatility and Program Continuity and Focus

Fluctuations in federal research appropriations and allocation of funds to specific mission-driven priorities are common across the research and development enterprise. Such fluctuations have consequences for universities; national laboratories; and the faculty, staff, and graduate students who rely on those funds. Respondents across BSSD and EESSD noted that BER's national and international leadership is vulnerable to perceived and realized uncertainties and volatility in funding, research priorities, and program continuity. Consistency in funding and strategic vision is required to maintain scientific focus, core infrastructure, and intellectual capabilities and to ensure sufficient longevity of research directions for career and workforce development.

Recent rapid shifts in topical priorities and the budgetary volatility they introduce pose challenges to sustain and grow BER leadership. One artifact of these issues has been significant program manager turnover requiring the addition of new program managers and subsequent changes in perspectives, priorities, and project assignments. Because relationships with program managers and knowledge of strategic priorities are important in understanding current and future research directions, time and energy are needed to become acquainted with new personnel. The pandemic and lack of in-person annual PI meetings have complicated such endeavors recently. As part of a holistic communications strategy, BER might consider having new program managers give introductory webinars to the research community.

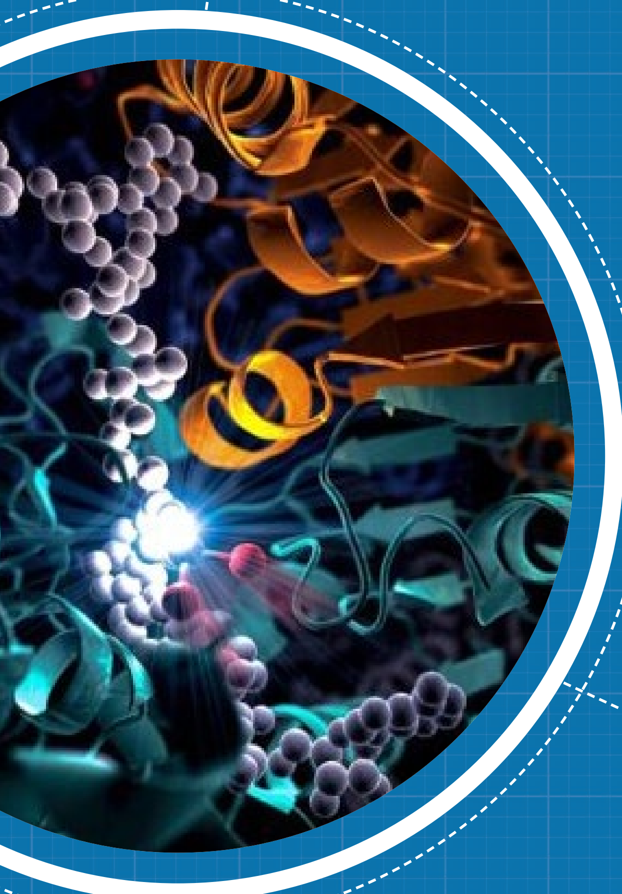
Although not readily apparent in annual funding cycles and budget allocations, perceived uncertainty and short-term fluctuations can impede BER science missions. Uncertainty resulting from changes of administration, presidential priorities, and changing research foci negatively impact hiring, retention, commitments to students and postdocs, and national laboratory investments. This uncertainty also reduces the willingness of scientists to fully engage in research areas no longer perceived as federal priorities and thus vulnerable to cuts. In short, the anticipation of change, whether it occurs or not, can hinder scientific commitment and progress. These perceptions and concerns are not short-lived within a given funding cycle, even if worst-case programmatic budgets are not realized; they are impacting BER's national and global reputation of supporting scientific careers and critical research for society.

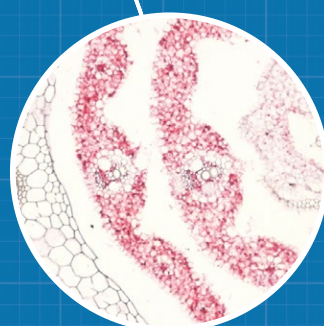
8.3.3 Horizon Scanning

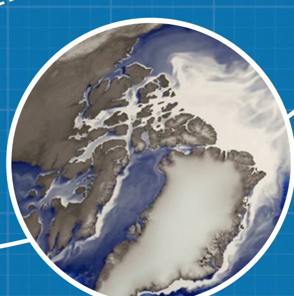
BER emphasizes a research community approach in generating workshop reports and convening roundtables to identify research questions and priorities, a strategy applauded by respondents and BERAC. The program also asks the National Academies of Sciences, Engineering, and Medicine to undertake independent consensus study reports. However, as the research enterprise becomes increasingly globalized, BER needs mechanisms to increase its agility in responding to breakthrough discoveries, reconfiguring its research portfolio, and translating fundamental science to technological innovation. The program could take advantage of proven methodologies for horizon-scanning exercises and scenario planning (NASEM 2000). Also, in a global research community, science is interdependent on others for success. Thus, it is critically important that BER communicate regularly with its international counterparts.

In summary, BER science and infrastructure are world-leading in scale and scope. BER mission areas have critical roles at the nexus of global challenges related to climate change, energy transitions, and sustainable prosperity. Investment across these mission areas needs to keep pace with that of the international research community and better leverage integrative science across BER's portfolio. BER needs to frequently scan the horizon of scientific opportunities and priorities to avoid failures of inspiration and imagination.

CHAPTER 9
Reflections and Conclusions







Subcommittee Co-Chairs
Maureen McCann, *National Renewable Energy Laboratory*
Patrick Reed, *Cornell University*

9 Reflections and Conclusions

DOE's origin story is rooted in response to national needs. The agency evolved from its first iteration in 1946 as the U.S. Atomic Energy Commission, which assumed leadership of the Manhattan Project after World War II, to its 1974 reinvention during the energy crisis as the U.S. Energy Research and Development Administration, tasked with developing new energy technologies. Ultimately, in 1977, President Jimmy Carter's administration drew an equivalency between energy security and national security and formed DOE to unite these two missions under a new federal agency.

Similarly, DOE's BER program began in 1947 under a different name and has evolved since then to become an international leader in diverse fields relevant to DOE missions. In the 1950s, BER contributed to studies of chemical dispersion, atmospheric global circulation, and environmental remediation of nuclear waste. By 1987, BER had partnered with the National Institutes of Health to sequence the human genome, partly to understand the impacts of radiation on DNA but also to develop the capability to sequence any organism's genome. In the 2000s, BER responded to DOE's intention to transform the nation's energy system and secure leadership in clean energy technologies; pursue world-class science and engineering as a cornerstone of economic prosperity; and enhance nuclear security through defense, nuclear nonproliferation, and environmental efforts. Toward those goals, BER research has increased understanding of biological systems and Earth and environmental systems. Due to these efforts, BER now occupies a unique position in the global scientific funding landscape at the nexus of energy transition, climate change mitigation, and sustainable economic prosperity.

This report reflects the BERAC Subcommittee on International Benchmarking's dedication to addressing the Office of Science director's four charge questions (see charge letter, p. ii), an effort requiring 40 colleagues to commit themselves to a task encompassing more than a year of their time. From the subcommittee to the many experts who provided a wealth of input, the scientific community's engagement and enthusiasm for this effort signifies deep respect for how BER manages and operates its research enterprise to support DOE missions. On the global stage, respondents provided unequivocal evidence of BER's international leadership across its mission areas. In developing this study, the subcommittee and its colleagues became enriched by a new appreciation for BER's practices, structures, protocols, resource investment, and scientific outcomes.

Across the various mission areas, the subcommittee identified five strategic recommendations and associated risks for the next decade:

1. If our nation *fails to invest* adequately in transformative and use-inspired discovery science, it risks undermining future capabilities to mitigate climate change impacts, manage energy transitions, and promote an emerging bioeconomy enabled by recombinant DNA technology. The integration of science across BER mission space in a true systems approach is an opportunity to amplify and accelerate progress.

2. If BER and DOE *fail to capitalize on investments* in translating fundamental science to market, they risk the international competitiveness of U.S. companies in the sectors of energy, agriculture, chemicals and materials, carbon capture technologies, and associated data and services.

3. If BER and DOE *fail to imagine* the consequences of science and innovation trajectories, they risk other nations reaping the benefits of technologies that drive step changes in the global economy. As the pace of discovery accelerates across the life sciences, regular horizon scanning is critical to ensuring that BER makes informed investments in research and infrastructure to remain at the forefront.

4. If BER and DOE *fail to inspire* their stakeholders and the public, they risk diminished stature and impact at a juncture when communicating the benefits of science in addressing societal needs is critical.
5. If BER and DOE *fail to sustain future leadership* through recruitment and retention of the best and brightest in the BER mission space, they risk the nation's international leadership in biological, environmental, and Earth systems science.

Given the urgency of addressing societal grand challenges by using "Big Science" to drive solutions, failure is not an option.

Maureen McCann and Patrick Reed
Co-Chairs, BERAC Subcommittee on International Benchmarking

September 2022

Appendix A

Key Findings and Recommendations

The BERAC Subcommittee on International Benchmarking developed both overarching and science domain–specific Key Findings and Recommendations based on their work to address the DOE Office of Science charge, which entailed synthesizing responses from expert interviews, town hall participants, and a public Request For Information. Data and analyses for these findings and recommendations were gathered and developed in 2021. BER has independently acted in some cases during 2022 to address some of the issues raised.

Overarching Findings

- BER's international leadership is well-substantiated across mission areas and enabling infrastructure.
- Mission areas increasingly target the critical challenges of the coming decades for which "Big Science" can and must be entrained.
- International leadership is a more meaningful goal when viewed in a collaborative versus adversarial context.
- Future leadership is not guaranteed and will require increased investments and strategic partnerships with private, public, and academic institutions; other DOE programs; other federal agencies; international collaborators; and across disciplines.
- Volatility in priorities, funding, and workforce retention significantly threatens BER's ability to sustain its leadership.
- BER's funding over the last decade has not increased commensurately with the growing scale and acuteness of the national and global challenges that BER missions and science address.
- The science community does not widely associate BER with the major research impacts and achievements it has enabled.

Strategic Recommendations

- Increase and sustain needed resources in all mission areas and in integrative science opportunities across and between these areas (risk: failure to invest).
- Improve connection between basic science and research across Technology Readiness Levels (risk: failure to capitalize on investment).
- Establish horizon-scanning mechanisms for long-range, strategic infrastructure and mission-area investments (risk: failure of imagination).
- Elevate the stature of BER mission science to ensure recruitment of the best and brightest (risk: failure to inspire).
- Prioritize, with time and investment, a culture that supports diversity and inclusion, enables early and mid-career professional development, and delivers the future workforce (risk: failure to sustain future leadership).

Ch. 2: Bioenergy and Environmental Microbiomes

Key Findings

KF2.1 BER is an international leader in fundamental bioenergy, sustainability, and environmental microbiome research, but other countries are catching up to the United States in scientific leadership and their capacity to translate basic research into practical applications.

KF2.2 BER funding of plant science studies has positioned the United States as the world leader in plant bioenergy and feedstock research.

KF2.3 BER leads in developing and applying genome- and omics-based approaches to bioenergy and environmental microbiome research. Maintaining this position requires continued support for new technologies and experimental testing of hypotheses generated from omics data. The next frontier will be combining multiomics approaches with innovations in microbial and plant biochemistry, areas where BER may lag other countries.

KF2.4 Several nations, including China, outperform the United States in developing and deploying technological applications, partly due to external policies and market trends, lower investment in fundamental bioprocessing research, and gaps in continuity between discovery, development, and deployment.

KF2.5 The DOE Bioenergy Research Center (BRC) program exemplifies the power of well-managed team science, which benefits from stable funding, a strong mission, and a collaboration emphasis. With well-integrated, multidisciplinary teams, the BRCs excel at performing and publishing research in foundational science and building collaborator networks, but their intellectual property has not been widely deployed.

KF2.6 Interagency calls, when initiated, provide a productive mechanism for fostering research collaborations.

Recommendations

R2.1 Spearhead a renaissance in bioenergy research, the need for which is highlighted by recent geopolitical events including the war in Ukraine and U.S. economic vulnerability to disruptions in the global energy market. To maintain its international position as a research leader, BER should support and encourage the next generation of researchers to embrace innovative, high-risk approaches for achieving bioenergy goals.

R2.2 Lead efforts to provide the fundamental knowledge needed to bring products to market. BERAC does not recommend that BER support applied research, since BER's strength and preeminence lie in fundamental science. However, BER should engage in creative opportunities to catalyze communication between basic and applied researchers to speed transitions between early Technology Readiness Levels.

R2.3 Encourage interactions and interdisciplinary collaborations that better integrate the unique architecture of BER's research portfolio and provide the research community with access to established resources such as ongoing perennial field experiments and their growing data collections. These activities will generate knowledge between and across disciplines and experimental scales, from computation to experimentation and from molecules to phenotypes.

R2.4 Build on genome-enabled bioenergy and environmental microbiome leadership and knowledge to understand the complex interactions between bioenergy crops and environmental microbiomes, thereby informing sustainable management of ecosystems under climate change.

Ch. 3: Biosystems Design

Key Findings

KF3.1 The relatively recent launch of BER's Biosystems Design research program is already yielding high-profile research accomplishments.

KF3.2 BER holds a strong leadership position in microbial biodesign, particularly in bacterial systems. However, leadership is increasingly distributed across the globe, with the United States considered "one of many" leaders for yeast and other fungi.

KF3.3 BER does not lead in understanding microbial physiology during bioprocess scale-up.

KF3.4 No world region yet leads in plant biodesign, suggesting that BER could target investments to yield substantial intellectual returns.

Recommendations

R3.1 Establish new Biodesign Research Centers patterned off existing DOE Bioenergy Research Centers to leverage advancements in BER's

Biosystems Design research, which encompasses multiple applications and could potentially synergize various biological platforms, including nonmodel and photosynthetic microbes.

R3.2 Explore and coordinate joint funding calls with international agencies to accelerate progress in biodesign by leveraging key expertise from other countries.

R3.3 Encourage replication of recent machine-learning breakthroughs, such as AlphaFold 2.0, and development of new deep-learning algorithms more broadly in biodesign. Target funding for curating, mining, and generating omics datasets and developing laboratory automation tools for generating high-quality datasets to train machine-learning models that support biodesign.

R3.4 Invest in disruptive, bold initiatives to accelerate plant synthetic biology and plant transformation processes in coordination with the National Science Foundation and other agencies.

R3.5 Expand support for biomanufacturing training programs for doctorate and nondoctorate workforces that critically feed the talent pipeline for the U.S. biotechnology industry.

Ch. 4: Environmental System Science

Key Findings

KF4.1 BER's Environmental System Science (ESS) research program is highly cited and internationally respected for its:

- **a.** Multidisciplinary systems science.
- **b.** ModEx (modeling-experimental) approach that emphasizes an iterative exchange of knowledge and discovery among predictive models, experiments, and observational field research, leading to novel discoveries.
- **c.** Research infrastructure, including large-scale ecosystem manipulations such as the Spruce and Peatland Responses Under Changing Environments (SPRUCE) project, AmeriFlux, and watershed Science Focus Areas, which support cross-agency and international collaboration.
- **d.** Terrestrial Ecology research, including biogeochemistry, ecosystem fluxes, and climate change responses.
- **e.** Watershed Sciences research, including multiscale hydro-biogeochemical modeling and process studies.

KF4.2 ESS research has untapped potential for:

- **a.** Better integrating human influence into the study of natural systems.
- **b.** Supporting both creative discovery science and the translation of research to inform applied solutions.
- **c.** Bridging the gaps between terrestrial sciences and atmospheric and climate sciences.

Recommendations

R4.1 Embrace coupled human-natural systems as a critical niche for ESS contributions in the next decade while maintaining the focus on mechanisms and process understanding.

R4.2 Elevate and integrate tools for data discovery and analysis at a level commensurate with ESS data volume and complexity to accelerate scientific impact.

R4.3 Facilitate the translation of ESS research into solutions and innovations by the DOE offices with a mandate for applied work and other potential partners.

R4.4 Create avenues for the research community to communicate and interact across the DOE science and technology pipeline, leading to breakthroughs, greater inclusivity, improved efficiencies, and reduced time lags between needs assessment, fundamental science, and application.

R4.5 Become an international leader in providing safe and inclusive fieldwork by building on existing ESS accomplishments, developing and sharing ESS resources, and modeling the successes that arise from equitable professional environments.

R4.6 Maintain global leadership in large-scale ecosystem manipulation experiments, a hallmark of BER science, which integrate ESS domains, promote ModEx, and foster collaboration among domestic and international institutions.

R4.7 Ensure that ESS strategic priority and funding paradigms support foundational research opportunities to continue international domain leadership.

Ch. 5: Climate Science

Key Findings

KF5.1 BER-funded climate science publications are among the most highly cited papers in the field, garnering a higher rate of citations than non-BER publications, particularly for the top 1% and 5% of papers.

KF5.2 BER has demonstrated international leadership in developing and interpreting climate model intercomparisons through the DOE Program for Climate Model Diagnosis and Intercomparison (PCMDI) and was a leading contributor to research earning the 2007 Nobel Peace Prize awarded to the Intergovernmental Panel on Climate Change and former U.S. Vice President Al Gore.

KF5.3 BER is a world leader in climate change and cloud feedback research through its application of the "fingerprint" method to identify signatures of human influence on climate and its development of innovative techniques to quantify cloud feedbacks and pin down equilibrium climate sensitivity.

KF5.4 BER has advanced exascale computing to become one of the world's leading developers of kilometer-scale Earth system models, such as the convection-permitting Energy Exascale Earth System Model.

KF5.5 BER has successfully developed capabilities in crosscutting energy-related research and coupled human-Earth system models, such as the Global Change Analysis Model.

KF5.6 BER leads internationally in capturing ground-based and aerial atmospheric measurements through its Atmospheric Radiation Measurement (ARM) user facility and in advancing physical understanding of atmospheric systems through the associated Atmospheric System Research program.

Recommendations

R5.1 Increase investment in development of kilometer-scale Earth system modeling by advancing exascale computing, artificial intelligence and machine-learning approaches, and model-observation integration.

R5.2 Strengthen international leadership in modeling the coupled human-Earth system by providing more decision-relevant insights and better accounting for model uncertainties.

R5.3 Sustain international leadership in ground-based and aerial measurements and their use in advancing physical process understanding by strengthening collaborations with the satellite community, supporting integration of national and international field-observing systems, and potentially establishing synergistic leadership in laboratory chamber facilities.

R5.4 Strengthen international leadership in model intercomparison activities and in climate sensitivity research by increasing support for PCMDI, the Earth System Grid Federation, and process-oriented exercises that use ARM observations.

R5.5 Establish sustained and substantial funding for expanded collaboration between U.S. agencies and universities to improve research outcomes and integration of efforts to meet societal needs.

R5.6 Create additional means for supporting "blue sky" proposals from DOE scientists to stimulate innovation and workforce engagement.

Ch. 6: Enabling Infrastructure

Key Finding

KF6.1 The review showed that BER research is currently supported by six world-class infrastructure capabilities:

a. **DOE Joint Genome Institute (JGI).** BER's JGI is the world's largest center for non-biomedical genomic science research, supporting DOE missions in clean energy and environmental characterization and cleanup. It provides integrated high-throughput sequencing and computational analysis that enable systems-based approaches to these challenges.

b. **Atmospheric Radiation Measurement (ARM) User Facility.** BER's ARM is internationally recognized for its long-term ground-based observation facilities, which have been advancing global atmospheric and climate research for 40 years. ARM's long-term data records, breadth of conditions and locations over diverse climate-relevant areas, and influence in the study of the climate system are unmatched by any other ground-based programs around the world.

c. **AmeriFlux and the AmeriFlux Management Project.** BER-supported AmeriFlux is a collection of long-term, eddy flux stations that measure ecosystem carbon, water, and energy fluxes across the Americas. One of two leading global flux networks, AmeriFlux is part of the international FLUXNET project and has taken the lead in creating the FLUXNET synthesis data products, the most impactful international observational product.

d. **National Synchrotron Light Source II (NSLS-II).** Supported by DOE's Office of Basic Energy Sciences, NSLS-II is the newest and most advanced synchrotron in the United States. The facility's design optimizes the creation of tightly collimated, high-flux light beams, covering the spectral range from infrared to high-energy X-rays. This unique combination of performance characteristics has allowed the creation of world-leading instruments, such as imaging with high spatial resolution (~10 nm) and chemical sensitivity, opening up novel possibilities for the study of biological material dynamics. Additional BER co-funded instruments with small beams (1 µm) are enabling high-resolution structural information from tiny protein crystals.

e. **DOE Leadership Computing Facilities.** Supported by DOE's Advanced Scientific Computing Research program, the Argonne Leadership Computing Facility, Oak Ridge Leadership Computing Facility (OLCF), and National Energy Research Scientific Computing Center are critical parts of the enabling infrastructure on which BER scientists rely. In June 2022, the high-performance computing community's international benchmarking effort ranked OLCF's Frontier supercomputer as the fastest in the world after it became the first system to break the exascale barrier. What distinguishes these DOE systems from international comparators is the science support ecosystem around them, provided by the DOE Exascale Computing Project (ECP). BER science has benefited from ECP in both its climate (Energy Exascale Earth System Model) and biology (ExaBiome) research.

f. **Environmental Molecular Sciences Laboratory.** EMSL delivers leading facilities, advanced instrumentation, and scientific leadership that empower and enable a national and international community of researchers to advance BER's mission to achieve a predictive understanding of complex biological, Earth, and environmental systems.

Recommendations

R6.1 Establish an oversight board to assess strategic decisions about creating, continuing, and sunsetting all BER infrastructure capabilities. This board should develop and publish a regularly updated 5- to 10-year strategic roadmap for infrastructure capabilities that support mission-critical science, coordinating with other DOE offices and national and international agencies to maximize investment and impact.

R6.2 Promote greater integration across user facilities—including harmonization of data management and analysis services—to enable researchers to easily schedule and use different infrastructure capabilities.

R6.3 Consider creating data user facilities and providing long-term support for their governance, planning, policy development, and technological needs.

R6.4 Establish a cross-facility working group to develop and share a foundational BER data policy and best practices for data use, licensing, and citation.

R6.5 Increase computational and storage capacity for BER researchers.

Ch. 7: Integrative Science

Key Findings

KF7.1 BER leads internationally in integrating climate observations and modeling, and its Atmospheric Radiation Measurement (ARM) user facility and Atmospheric System Research (ASR) program are international leaders of integrative science involving short-term field campaigns.

KF7.2 Sustaining leadership in the integration of the ARM, ASR, and Earth system modeling programs requires both maintenance of cutting-edge observational capabilities and continued access to adequate computational resources.

KF7.3 Additional leadership gains would be achieved by improving integration across the Energy Exascale Earth System Model (E3SM), the Program for Climate Model Diagnosis and Intercomparison, research in Regional and Global Model Analysis, ARM, and MultiSector Dynamics modeling efforts.

KF7.4 The DOE Bioenergy Research Centers (BRCs) exemplify interdisciplinary research ranging from detailed molecular analysis to ecosystem modeling.

KF7.5 DOE's Environmental Molecular Sciences Laboratory (EMSL), Joint Genome Institute (JGI), and light source user facilities, along with their numerous collaborators, are international leaders in integrating omics research, molecular and structural analysis, and systems biology.

KF7.6 BER is a leader in systems-level understanding such as the linkages between plant microbiomes and ecosystem function.

KF7.7 EMSL successfully integrates atmospheric science and physical chemistry with potential expansion into biological aerosols.

KF7.8 Citation analysis demonstrates integration success: BER-sponsored papers are 1.5 times more likely than non-BER papers to span two BER science areas and 3 times more likely to span three.

KF7.9 BER research could be further integrated by developing opportunities embodied in crosscutting user facility programs such as the Multidisciplinary drifting Observatory for the Study of Arctic Climate (MOSAiC) project and the Facilities Integrating Collaborations for User Science (FICUS) initiative.

KF7.10 Integrating efforts across U.S. agencies is a formidable challenge leaving unrealized opportunities for further integration across BER's portfolio.

Recommendations

R7.1 Improve BER's capacity for integrative research within and beyond its research portfolio.

a. Solicit support from the National Academies of Sciences, Engineering, and Medicine for synthesizing capabilities, needs, and opportunities across BER-relevant user facilities and field sites funded by DOE and other U.S. agencies to accelerate groundbreaking integrative research.

b. Create sustained funding opportunities across BER, DOE, and other agencies (where possible) to advance a more integrated understanding of biological and environmental systems at multiple scales.

c. Strengthen workforce capacity for integration by better supporting integrative research with targeted funding opportunities, particularly among early career researchers.

R7.2 Advance a more complete understanding of coupled human-natural systems in BER science areas.

a. Include coupled human-natural system dynamics in BER funding opportunities.

b. Launch a multiagency research program to improve integration across both the MultiSector Dynamics and Earth and Environmental Systems Modeling programs.

c. Establish research sites for integrated long-term studies that span genomes to landscapes and the subsurface to atmosphere.

R7.3 Build international collaborations to strengthen BER's global leadership in the genomic, environmental, and climate modeling sciences.

a. Work jointly with other U.S. agencies to develop an internationally coordinated effort that will provide public and private stakeholders with urgently needed climate and environmental data.

b. Explore the potential for coordinating and promoting international collaborations that would leverage BER's investments in the genomic and environmental sciences, including the BRCs.

R7.4 Support integration through existing and new user facilities.

a. Establish a computational synthesis center to support the pursuit of questions that demand targeted integration across disciplines and scales.

b. Dedicate a cross-facilities operational budget to fund integrative science projects spanning multiple BER user facilities.

Ch. 8: Strategies for People, Partnerships, and Productivity

Key Findings

PEOPLE

KF8.1 BER funds academic scientists across the nation who contribute exceptional talent and new expertise to the program's mission.

KF8.2 The DOE national laboratory complex provides many positive career opportunities for BER-funded scientists.

KF8.3 Programs for undergraduates, graduate students, and postdoctoral students effectively recruit scientific talent for BER missions.

KF8.4 The lack of workforce diversity significantly limits BER's long-term leadership and the necessary growth of its scientific workforce.

KF8.5 BER frontier research successes and impacts lack visibility.

KF8.6 BER funding for high-risk discovery science and paths to independent work are rare at the national laboratories, and increased funding flexibility is desired at all career levels.

KF8.7 Real and perceived volatility in funding levels and research topics hampers workforce recruitment and retention at all career stages and impedes long-term productivity.

KF8.8 Current funding models produce high levels of professional anxiety among national laboratory programmatic staff who feel pressure to continuously secure projects that support their own salaries.

KF8.9 At some user facilities, limited opportunities exist for support staff advancement, independent research, and future career choices, leading to overwork and professional burnout. These challenges vary significantly depending on the operational model of a given facility.

KF8.10 Over the last decade, BER has seen attrition of scientific workforce talent, particularly among academic Early Career Research Program awardees, half of whom are no longer funded in the BER mission space.

KF8.11 Some BER-supported Early Career awards are limiting workforce development due to their timing and topical volatility, providing only narrow windows of opportunity in a scientist's career pathway. This impact is more pronounced for the Earth and Environmental Systems Sciences Division than the Biological Systems Science Division and its more stable approach.

PARTNERSHIPS

KF8.12 Although international collaborations are critical for strengthening BER scientific output and increasing global visibility, such partnerships are difficult for BER-funded institutions due to funding restrictions between countries.

KF8.13 BER program staff and BER-supported scientists have few resources to travel or engage internationally.

KF8.14 Meeting societal needs requires more domestic and international collaborations for ground-based observations and high-resolution Earth system modeling to improve research outcomes and ensure integration of efforts.

KF8.15 Because of its mobile facilities and ability to fund international partners, the Atmospheric Radiation Measurement (ARM) user facility excels in collaborations—both in the United States and abroad.

PRODUCTIVITY

KF8.16 BER user facilities are specially positioned to integrate researchers across BER because of their unique expertise, leadership positions, and ability to attract users.

KF8.17 The Bioenergy Research Center (BRC) program achieves strategically important BER mission goals, and its model could be applied to other relevant research areas, such as environmental microbiomes. With their integrative focus, the BRCs have excelled at building impactful and highly productive researcher networks working toward a common goal.

KF8.18 BER should maintain team-based projects combining researchers from academic institutions and DOE national laboratories.

KF8.19 Silos and mission boundaries within DOE and across agencies block the potential for science accomplishments to inform innovation and applied solutions.

KF8.20 U.S. agencies should consider opportunities to expand collaborative climate science research beyond the current facilitating role of the U.S. Global Change Research Program, which lacks allocated funding.

Recommendations

PEOPLE

R8.1 Incentivize efforts to increase workforce diversity and provide a culture of inclusivity, explicitly measuring successes and evaluating outcomes continually for further improvements using processes with broad participation.

R8.2 Invest in effectively communicating BER scientific successes and proactively convey the importance of the program's research mission to better recruit and retain top global talent.

R8.3 Support Early Career award researchers in their future and post-award career paths by providing training and opportunities for research leadership.

R8.4 Provide incentives to the national laboratories for creating and sustaining professional development opportunities for early and mid-career scientists.

R8.5 Develop and demonstrate balanced models for providing BER-supported researchers with options for both collaborative teaming paths and individual successes.

PARTNERSHIPS

R8.6 Enhance international partnerships and cross-agency cooperation by developing new funding modalities, such as joint calls with the National Science Foundation and other agencies.

R8.7 Increase opportunities for BER program managers and supported scientists to engage with their international counterparts.

R8.8 Develop new international programs and consider establishing a formal office for international activities.

R8.9 Increase fellowships, scholarships, and international exchange opportunities.

R8.10 Optimize resources and efficiencies by bridging across agencies and nations.

PRODUCTIVITY

R8.11 Promote more effectively BER's world-class programs; unique facilities; and leadership in creating synergies across observations, process studies, and system modeling.

R8.12 Secure leadership in both the science areas where BER already excels (e.g., observation and modeling integration) and in new growth areas.

R8.13 Assign facilities the responsibility of coordinating and storing the data relevant to their main area of expertise.

R8.14 Increase emphasis in modeling activities related to uncertainty quantification and uncertainty propagation for complex, multiscale systems.

R8.15 Build a productive, creative workforce by supporting interdisciplinary research opportunities for early and mid-career scientists, as is done by crosscutting organizations such as the Max Planck Institutes in Europe or Chinese institutes for environmental and climate science.

R8.16 Manage volatility, potential and realized, in funding levels and award topics.

R8.17 Use inter- and intra-agency cooperation and co-funding to foster interdisciplinary collaborations, maximize large-scale resources, and bridge Technology Readiness Levels (TRLs).

R8.18 Create a culture of communication and interaction across the TRL spectrum in DOE and among BER, businesses, and nongovernmental organizations.

R8.19 Develop integrative science opportunities as a signature area for BER.

Appendix B
BERAC Members

Chair
Bruce Hungate, *Northern Arizona University*

Members
Caroline Ajo-Franklin, *Rice University*
Cris Argueso, *Colorado State University*
Sarah M. Assmann, *Pennsylvania State University*
Ana P. Barros, *University of Illinois*
Bruno Basso, *Michigan State University*
Julie S. Biteen, *University of Michigan*
Sen Chiao, *Howard University*
Leo Donner, *Princeton University*
Robert F. Fischetti, *Argonne National Laboratory*
Matthew Fields, *Montana State University*
Ann M. Fridlind, *NASA Goddard Institute for Space Studies*
Jorge E. Gonzalez-Cruz, *City College of New York*
Ramon Gonzalez, *University of South Florida*
Randi Johnson, *Formerly U.S. Department of Agriculture*
Kerstin Kleese van Dam, *Brookhaven National Laboratory*
Sonia Kreidenweis, *Colorado State University*
Maureen McCann, *National Renewable Energy Laboratory*
Xiaohong Liu, *Texas A&M University*
Gerald A. Meehl, *National Center for Atmospheric Research*
Gloria K. Muday, *Wake Forest University*
Dev Niyogi, *Jackson School of Geosciences*
Himadri Pakrasi, *Washington University in St. Louis*
Kristala Prather, *Massachusetts Institute of Technology*
Patrick Reed, *Cornell University*
Gemma Reguera, *Michigan State University*
Jeremy Schmutz, *Hudson Alpha Institute for Biotechnology*
Daniel Segrè, *Boston University*
Karen Seto, *Yale University*
Matthew D. Shupe, *University of Colorado and NOAA*
Huimin Zhao, *University of Illinois at Urbana-Champaign*

Appendix C
Approach to Metrics and Methodologies

We are deeply grateful to Tristram West, our guide within this report and to BER; to AAAS fellow Wayne Kontur, on detail at BER; and to Mary Beth West and Joshua Nelson from DOE's Office of Scientific and Technical Information.

Methodology for Publication and Citation Analysis

The BERAC subcommittee performed a quantitative assessment of BER-focused research, resulting publications, and citation metrics to assess the relative impact of BER-sponsored research. This quantitative research analyzed publications and citations from Clarivate's Web of Science (WoS) Expanded Application Programming Interface (API). WoS is an independent global citation database with almost 1.9 billion cited references from over 171 million records.

Bibliometric analysis is one method to determine the relative impact of a publication. For this research, the BERAC subcommittee assessed the citation activity of relevant publications to compare BER-related research. Similar reporting activities[1] have used citation-based bibliometrics to support scientific and scholarly comparisons.

For this study, the evaluation dataset was composed of journal articles published between 2010 and 2020. The final queries were pulled from the WoS Expanded API in mid-March 2022.

Comparison groups (e.g., BER, U.S./domestic, and non-U.S./international) were identified via funding information and author affiliations as follows:

- **BER:** If a publication's funding agency, funding details, or funding text fields contain "BER," "Biological and Environmental Research," or "Biological and Environmental Research," a publication is considered to be in the BER comparison group.
- **U.S./domestic:** If a publication's authorship contains U.S. affiliations, a publication is considered to be in the U.S. comparison group. This is consistent with how country facets are identified in WoS front-end search analyses.
- **Non-U.S./international:** If a publication falls into neither of the first two categories, it is considered to be in the non-U.S. comparison group.

The subcommittee scoped and iterated through a three-phase data aggregation and analysis approach to support quantitative comparisons of BER-sponsored research compared to domestically and internationally funded research. To characterize the research areas, each working group identified relevant domain-specific subjects and keywords that represent BER research and could be applied to assess domestic and international research. WoS API queries were developed using each working group's keywords.

Phase One Methodology

For the first research phase, the subcommittee identified suitable comparison metrics, identified BER's Science Focus Areas[2] (SFAs) as a method to derive initial subject areas, and developed a method for acquiring and analyzing the publication and citation metadata.

Development of the initial set of BER SFA-focused WoS queries involved combinations of manual and automated keyword lists. These WoS queries were used to perform an exploratory assessment of relevant publications, inform the scoping of future phases, and provide preliminary comparative metrics using "average citation per publication" as a baseline metric.

BER's SFAs were used to characterize distinct areas of research for comparison purposes, which were later grouped into discrete concepts. For each SFA, high-level keywords were compiled based on a manual

[1] science.osti.gov/-/media/bes/pdf/reports/2021/International_Benchmarking-Report.pdf

[2] science.osti.gov/ber/Funding-Opportunities/L y-Scientific-Focus-Area-Guidance

review of past funding opportunity announcements[3] (FOAs). Additional keywords were aggregated through comparison activities, during which SFA text descriptions were compared to publications in Microsoft Academic Graph[4].

Using a Gensim/Doc2Vec model, which was trained on more than 80 million English language publications, each SFA description was associated with Microsoft Knowledge Graph[5] (MKG) knowledge labels from domain-relevant publications. These sets of knowledge labels were further curated by subject matter experts in each working group and used to further expand and adjust the Phase One WoS queries.

Phase Two Methodology

The BERAC subcommittee reviewed the generated Phase One WoS queries, the aggregated publication lists, and the resulting metrics to inform Phase Two's quantitative evaluation.

In the first phase, BER SFAs were used to delineate concept areas for exploratory query development and comparison. In the second phase, concept areas were realigned around the working group research areas; this shift more directly aligned with this report's charge letter. The exploratory SFA queries were mapped to working groups where appropriate and, along with additional feedback from working groups in Phase One, were used as a basis for acquiring an initial publication dataset.

Author-supplied keywords and WoS subject labels were extracted from metadata in the initial dataset to identify additional concept labels characterizing working group research areas. Metadata was also matched against Microsoft Academic data to identify other relevant MKG labels. Aggregated term lists were provided to working groups for review and keyword gap analysis. Refined queries were developed with feedback from each working group, and these queries were used to pull a preliminary dataset for analysis, 2010–2020 inclusive, using the WoS Expanded API.

[3] science.osti.gov/ber/Funding-Opportunities

[4] www.microsoft.com/en-us/research/project/microsoft-academic-graph/

[5] makg.org

After comparing and aggregating available knowledge labels, a keyword gap analysis was performed, and the analysis was sent to each relevant working group. Each working group reviewed the analysis, and the keywords were refined into the appropriate WoS API queries, which were again reviewed by each working group.

Publications in the analysis dataset were separated into funding comparison groups (i.e., BER, U.S/domestic, and non-U.S./international) by referencing each publication's funding acknowledgments and author affiliations, as described above. Citation numbers were used to calculate benchmark metrics of representation in top citation percentiles and average citations per publication over the reporting period.

At the end of Phase Two, the WoS queries, all extracted publication metadata, and the aggregated results (e.g., comparative citation benchmark and analysis) were reviewed by each working group. Each working group performed data validation and analysis, which resulted in additional feedback to inform Phase Three query iteration and refinement.

Phase Three Methodology

During the last phase of quantitative data acquisition and analysis, the WoS queries were finalized, and this study's publications dataset was pulled from the WoS API in mid-March 2022.

To finalize the queries, each working group reviewed the Phase Two dataset (e.g., relevant WoS queries, citation analysis, etc.). Phase Two publication metadata were reviewed and compared against known BER, domestic, and international publication lists to identify gaps in concept coverage. To address coverage gaps, additional datasets associated with specific programs in funding acknowledgment or funding opportunities were also pulled and used for this purpose.

Finalized WoS queries to support benchmark metrics were reviewed and approved by the working groups. After the queries, the benchmark metric datasets were pulled and analyzed to compile final results.

Additional datasets and results beyond benchmark metrics were developed and provided on an as-needed basis in response to individual working group requests. These additional queries were developed for deeper analyses supporting specific narrative elements. In some cases, these analyses do not fall within the scope of this report but may inform later inquiries.

Chapter 6 Metrics

- Number of user groups and users
- Acknowledgments of use of the facility in publications
- Use of international facilities by BER researchers and vice versa
- For light and neutron sources, and cryo-EM facilities—number of Protein Data Bank deposits
- Development of new capabilities
- Facility utilization and level of subscription
- Outreach and dissemination metrics.

Chapter 7 Metrics

- Integrative science occurs in multiple dimensions—lab/fieldwork/modeling/theory within an area of research or across different areas of science
- Survey among leaders of integrative research activities
- Interdisciplinarity (multiple programs, multi-agency) of high-impact publications
- Synergistic collaborations across U.S. agencies and entities (numbers of projects)
- Mechanisms that allow national laboratories to collaborate

Final Web of Science Queries (Phase Three)

Working Group 2 Keyword Queries

"biosynthetic pathway*" or "metabolic engineering" or "synthetic biology" or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and (bacteria or microbe*)) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and "systems biology") or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("biosynthetic pathway*" or "pathway engineering")) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and (biofuel* or bioproduct* or biomaterial*)) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("genome engineering" or "genome-scale engineering" or "genome scale model*")) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and "microbiome engineering") or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or (("metabolic engineering" or "metabolic modeling" or "metabolic network" or "secondary metabolism") and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or ((bacteria or microbe*) and "systems biology") or ((bacteria or microbe*) and ("biosynthetic pathway*" or "pathway engineering")) or ((bacteria or microbe*) and (biofuel* or bioproduct* or biomaterial*)) or ((bacteria or microbe*) and ("genome engineering" or "genome-scale engineering" or "genome scale model*")) or ((bacteria or microbe*) and "microbiome engineering") or ((bacteria or microbe*) and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or ((bacteria or microbe*) and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or ((bacteria or microbe*) and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or ((bacteria or microbe*) and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or ("systems biology" and ("biosynthetic pathway*" or "pathway engineering")) or ("systems biology" and (biofuel* or bioproduct* or biomaterial*)) or ("systems biology" and ("genome engineering" or "genome-scale engineering" or "genome scale model*")) or ("systems biology" and "microbiome engineering") or ("systems biology" and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or ("systems biology" and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or ("systems biology" and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or ("systems biology" and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or (("biosynthetic pathway*" or "pathway engineering") and (biofuel* or bioproduct* or biomaterial*)) or (("biosynthetic pathway*" or "pathway engineering") and ("genome engineering" or "genome-scale engineering" or "genome scale model*")) or (("biosynthetic pathway*" or "pathway engineering") and "microbiome engineering") or (("biosynthetic pathway*" or "pathway engineering") and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or (("biosynthetic pathway*" or "pathway engineering") and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or (("biosynthetic pathway*" or "pathway engineering") and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or (("biosynthetic pathway*" or "pathway engineering") and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or ((biofuel* or bioproduct* or biomaterial*) and ("genome engineering" or "genome-scale engineering" or "genome scale model*")) or ((biofuel* or bioproduct* or biomaterial*) and "microbiome engineering") or ((biofuel* or bioproduct* or biomaterial*) and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or ((biofuel* or bioproduct* or biomaterial*) and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or ((biofuel* or bioproduct* or biomaterial*) and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or ((biofuel* or bioproduct* or biomaterial*) and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or (("genome engineering" or "genome-scale engineering" or "genome scale model*") and "microbiome engineering") or (("genome engineering" or "genome-scale engineering" or "genome scale model*") and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or (("genome engineering" or "genome-scale engineering" or "genome scale model*") and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or (("genome engineering" or "genome-scale engineering" or "genome scale model*") and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or (("genome engineering" or "genome-scale engineering" or "genome scale model*") and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or ("microbiome engineering" and ("adaptive laboratory evolution" or "directed evolution" or "rational design")) or ("microbiome engineering" and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or ("microbiome engineering" and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or ("microbiome engineering" and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or (("adaptive laboratory evolution" or "directed evolution" or "rational design") and ("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering")) or (("adaptive laboratory evolution" or "directed evolution" or "rational design") and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or (("adaptive laboratory evolution" or "directed evolution" or "rational design") and ("data exchange standard*" or "data infrastructure" or "data ontolog*")) or (("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering") and ("artificial intelligence" or "machine learning" or "multiscale model*" or "multi-scale model*")) or (("computational protein design" or "protein engineering" or "protein design" or "enzyme engineering") and ("data exchange standard*" or "data infrastructure" or "data ontolog*"))

Working Group 2 Funding Queries

BER or "Biological and Environmental Research" or "Biological & Environmental Research"

Working Group 3 Keyword Queries

(biomass or biofuel* or bioenergy or feedstock or ethanol) and (biorefinery or "metabolic engineering" or "synthetic biology" or *cellulos* or lignin or switchgrass or "corn stover" or arabidopsis or "enzymatic hydrolysis" or fermentation or genom* or genom* or "systems biology" or *omics or plant or microb*)

Working Group 3 Funding Queries

BER or "Biological and Environmental Research" or "Biological & Environmental Research"

Working Group 4 Keyword Queries

("environmental system*" and ecolog*) or ("environmental system*" and ecosystem*) or ("environmental system*" and hydrolog*) or ("environmental system*" and ("soil water" or "surface water" or watershed*)) or ("environmental system*" and "terrestrial ecosystem*") or ("environmental system*" and (biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community")) or ("environmental system*" and subsurface) or ("environmental system*" and soil) or (ecolog* and ecosystem*) or (ecolog* and hydrolog*) or (ecolog* and ("soil water" or "surface water" or watershed*)) or (ecolog* and "terrestrial ecosystem*")or (ecolog* and (biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community")) or (ecolog* and subsurface) or (ecolog* and soil) or (ecosystem* and hydrolog*) or (ecosystem* and ("soil water" or "surface water" or watershed*)) or (ecosystem* and "terrestrial ecosystem*") or (ecosystem* and (biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community")) or (ecosystem* and subsurface) or (ecosystem* and soil) or (hydrolog* and ("soil water" or "surface water" or watershed*)) or (hydrolog* and "terrestrial ecosystem*") or (hydrolog* and (biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community")) or (hydrolog* and subsurface) or (hydrolog* and soil) or (("soil water" or "surface water" or watershed*) and "terrestrial ecosystem*") or (("soil water" or "surface water" or watershed*) and (biogeochem* or biogeophys* orhydrobiogeochem* or "microbial community")) or (("soil water" or "surface water" or watershed*) and subsurface) or (("soilwater" or "surface water" or watershed*) and soil) or ("terrestrial ecosystem*" and (biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community")) or ("terrestrial ecosystem*" and subsurface) or ("terrestrial ecosystem*" and soil) or((biogeochem* or biogeophys* or hydrobiogeochem* or "microbial community") and subsurface) or ((biogeochem* or biogeophys*or hydrobiogeochem* or "microbial community") and soil)

Working Group 4 Funding Queries

BER or "Biological and Environmental Research" or "Biological & Environmental Research"

Working Group 5 Keyword Queries

((climat* or hydrolog* or ecosystem* or cloud*) and microphys*) or ((climat* or hydrolog* or ecosystem* or cloud*) and resilience) or ((climat* or hydrolog* or earth or ecosystem*) and "infrastructure system*") or ((climat* or hydrolog* or earth or ecosystem*) and "energy transition*") or "integrated assessment model*" or "energy-water-land" or "food-energy-water" or "climat* model*" or "hydrolog* model*" or "earth model*" or "earth system model*" or "ecosystem* model*" or "atmospher* (model* or simulation)" or "cloud resolv*" or (radiation cloud* atmospher*)

Working Group 5 Funding Queries

BER or "Biological & Environmental Research" or "Biological and Environmental Research" or "ARM" or "Atmospheric Radiation Measurement" or "ASR" or "Atmospheric System Research" or "RGMA" or "Regional and Global Model Analysis" or "ESMD" or "Earth System Model Development" or "RGCM" or "Regional and Global Climate Modeling" or "ESM" or "Earth System Modeling"

Appendix D
Request For Information
U.S. Department of Energy: Assessing the National and International Standing of BER Basic Research

Agency: Office of Science, Biological and Environmental Research Program, Department of Energy.

Action: Request For Information

Summary: The Biological and Environmental Research (BER) Program, as DOE's coordinating office for research on biological systems, bioenergy, environmental science, and Earth system science, is seeking input on technical and logistical pathways that would enhance the BER research portfolio in comparison to similar international research efforts.

Dates: Written comments and information are requested on or before October 31, 2021.

Addresses: Interested persons may submit comments by email only. Comments must be sent to BERACRFI@ science.doe.gov with the subject line "BER research benchmarking."

For further information, contact: Dr. Tristram O. West, (301) 903–5155, Tristram.west@science.doe.gov.

Supplementary information: A charge was issued from the Director of Office of Science on October 8, 2020, to the BER Advisory Committee (BERAC) to assess BER's standing in relation to related research efforts nationally and internationally, and to consider strategies that would increase BER's ability to conduct world-class science in core BER research areas. The Director's charge letter may be found here: https://science.osti.gov/ber/berac/Reports/Current-BERAC-Charges.

The information collected through this request, in addition to other informational sources, may be used by BERAC to develop strategies to further strengthen BER's research capabilities. The conclusions drawn from BERAC's effort are expected to serve as a benchmark for BER's standing in core research areas and provide strategies for improvement where appropriate.

Request For Information

The objective of this Request For Information is to gather information on BER's standing in relation to related research efforts occurring nationally and internationally, and how BER might increase its stature in conducting world-class basic science currently supported by BER (https://science.osti.gov/ber/Research). Supported research includes Atmospheric Science; Earth and Environmental System Modeling; Environmental Science; Bioenergy and Bioproducts; Plant and Microbial Genomics; Data Analytics and Management; and Scientific User-focused Infrastructure (i.e., DOE User Facilities, Computational Knowledgebase Platforms, Community Observational and Analytical Resources). Information is specifically requested on the status of current capabilities, partnerships, funding mechanisms, and workforce development specific to one or more of the aforementioned research areas. Answers or information related, but not limited, to the following questions are specifically requested:

- Within the BER-supported topical research areas and facility capabilities, in which areas and capabilities, presently or in the foreseeable future, does BER lead in the international community, and in which areas does leadership require strengthening? In identifying these areas, please consider their critical mission relevance, recent history, the status quo, observable trends, and evidence-based projections.
- Are there key international partnerships that could strengthen BER science output and increase global visibility of BER?
- Is there a preferred optimization for organizing research, collaboration, and funding mechanisms

among labs, universities, and other federal agencies to preserve and foster U.S. leadership with resource constraints? Are there other key efficiencies and balances that should be considered and modified to improve U.S. leadership in BER research areas?

- How can BER programs and facilities be structured and managed to create incentives that will attract and retain talented people deciding whether to pursue a scientific career, as well as mid-career scientists considering whether to stay in the U.S.?
- What are the key opportunities for BER in attracting and enhancing careers in BER-supported scientific fields?

While the questions provided above can help guide thinking on this topic, any input is welcome which may help DOE assess BER's international standing in the core research areas. The information provided through this request should be presented as specific strategies which DOE Office of Science could implement and track.

Signing Authority

This document of the Department of Energy was signed on August 11, 2021, by Dr. J. Stephen Binkley, Acting Director, Office of Science, pursuant to delegated authority from the Secretary of Energy. The document with the original signature and date is maintained by DOE. For administrative purposes only, and in compliance with requirements of the Office of the Federal Register, the undersigned DOE Federal Register Liaison Officer has been authorized to sign and submit the document in electronic format for publication, as an official document of the Department of Energy. This administrative process in no way alters the legal effect of this document upon publication in the Federal Register.

Signed in Washington, DC, on August 12, 2021.

Treena V. Garrett,
Federal Register Liaison Officer
U.S. Department of Energy
[FR Doc. 2021–17658 Filed 8–17–21; 8:45 am]
BILLING CODE 6450–01–P

Appendix E
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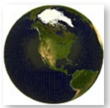
Appendix F

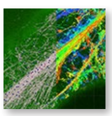
Image Credits

Executive Summary



Grid view of Earth from the atmospheric component of the Energy Exascale Earth System Model (E3SM). [Reprinted under a Creative Commons license (CC BY-NC-ND 4.0) from Rasch, P.J., et al. 2019. "An Overview of the Atmospheric Component of the Energy Exascale Earth System Model," *JAMES: Journal of Advances in Modeling Earth Systems* **11**(8), 2377-2411.]

Headwaters of Snake River. [Courtesy Environmental Molecular Sciences Laboratory]

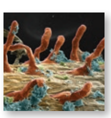


Plant protein dynamics. [Courtesy University of Delaware]

A soil-grown root system. [Courtesy Carnegie Institute for Science]

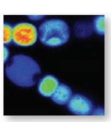
Chapter 1: Introduction

Researcher collects *Miscanthus* root samples. [Courtesy Center for Advanced Bioenergy and Bioproducts Innovation]



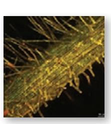
Magnified view of a red pine (*Pinus resinosa*) root and associated microbiome. [Courtesy Environmental Molecular Sciences Laboratory]

Modeled ice speed for the Antarctic ice sheet. [Courtesy Los Alamos National Laboratory]



Photobleached cell. [Courtesy University of Colorado–Boulder and University of Illinois–Chicago]

Chapter 2: Bioenergy and Environmental Microbiomes



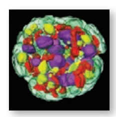
Microbes colonizing poplar roots. [Courtesy Oak Ridge National Laboratory]

Researchers sample soils to understand how climate change affects microbial growth efficiency and soil carbon stocks. [Courtesy University of Massachusetts–Amherst]

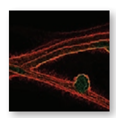
A sorghum field with bagged flowers to prevent pollen exchange. [Courtesy Lawrence Berkeley National Laboratory]

Plants at different stages of growth. [Courtesy Oak Ridge National Laboratory]

Chapter 3: Biosystems Design



Cryo-soft X-ray tomography of a reconstructed green alga cell. [From Roth, M.S., et al. 2017. "Chromosome-Level Genome Assembly and Transcriptome of the Green Alga *Chromochloris zofingiensis* Illuminates Astaxanthin Production," *PNAS* **114**(21), E4296-E4305.]



Transgenic roots of *Medicago truncatula* with nodules formed by its symbiont (*Sinorhizobium meliloti*). [Courtesy University of Florida]

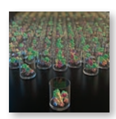


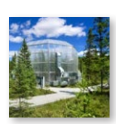
Illustration of engineered biosynthetic metabolic pathways. [Reprinted by permission from Springer Nature from Karim, A. S., et al. 2020. "*In Vitro* Prototyping and Rapid Optimization of Biosynthetic Enzymes for Cell Design," *Nature Chemical Biology* **16**(8), 912–19. Copyright 2020.]

Yeast strain *Yarrowia lipolytica*. [Courtesy University of Tennessee]

Chapter 4: Environmental System Science

East River watershed in upper Colorado River Basin. [Courtesy Lawrence Berkeley National Laboratory]

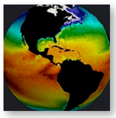
Catlett Islands water sediment site. [Courtesy Pacific Northwest National Laboratory]

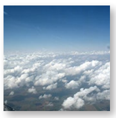


The Spruce and Peatland Responses Under Changing Environments (SPRUCE) research site located in northern Minnesota. [Courtesy Oak Ridge National Laboratory]


Next-Generation Ecosystem Experiments (NGEE) Tropics field site in Puerto Rico. [Courtesy Lawrence Berkeley National Laboratory]

Chapter 5: Climate Science


E3SM model of sea surface temperature. [Courtesy E3SM]


Fair weather clouds studied as part of the Cloud and Land Surface Interaction Campaign by the Atmospheric Radiation Measurement (ARM) user facility. [Courtesy ARM]

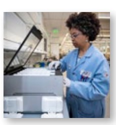

Road junction. [Courtesy Getty Images]

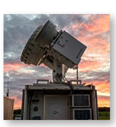

Instruments from ARM user facility's Cloud, Aerosol, and Complex Terrain Interactions (CACTI) field campaign in the Sierras de Córdoba mountain range of north-central Argentina. [Courtesy ARM]

Chapter 6: Enabling Infrastructure

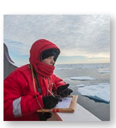

Magnified view of the mineral olivine forsterite. [Courtesy Pacific Northwest National Laboratory]

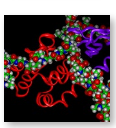

Ca-Ca3 AmeriFlux Tower in British Columbia. [Courtesy AmeriFlux]

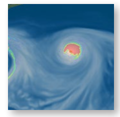

Researcher loads a DNA sequencer. [Courtesy Lawrence Berkeley National Laboratory]


ARM cloud radar in Brazil. [Courtesy ARM]

Chapter 7: Integrative Science


MOSAiC researcher. [Reprinted with permission from the Alfred Wegener Institute/Esther Horvath under a Creative Commons License.]

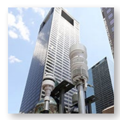

Computer simulations of the T4 lysozyme wrapped around a bacterial cell wall. [Courtesy Environmental Molecular Sciences Laboratory]


E3SM Category 5 hurricane simulation. [Courtesy E3SM]


Researcher working on lignin digestibility. [Courtesy Great Lakes Bioenergy Research Center]

Chapter 8: People, Partnerships, and Productivity

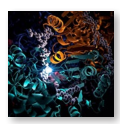

Researchers examine plant-microbe interactions to improve biomass feedstock growth. [Courtesy DOE Joint Genome Institute]


A mobile atmospheric observatory operating in downtown Houston [Courtesy ARM]

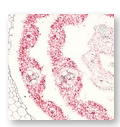

X-ray crystallographer analyzes SARS-CoV-2 proteins at the Advanced Photon Source. [Courtesy Argonne National Laboratory]

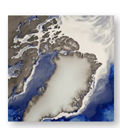

Sampling during the MOSAiC expedition. [Reprinted with permission from the Alfred Wegener Institute/Torsten Sachs under a Creative Commons License]

Chapter 9: Reflections and Conclusions


Artist interpretation of the enzyme enoyl-CoA carboxylase/reductase. [Courtesy SLAC National Accelerator Laboratory]


Section of the Columbia River watershed. [Courtesy Pacific Northwest National Laboratory]


BdTHX1 expression (red, immunolabeling) in the leaf sheath of *Brachypodium*. [Courtesy Great Lakes Bioenergy Research Center]


E3SM simulation of the Arctic Ocean showing surface ocean currents, temperatures, and sea-ice concentration. [Courtesy E3SM]

Appendix G

Acronyms and Abbreviations

3CLpro	3 chymotrypsin-like protease
AAF	ARM Aerial Facility
AcceLNet	Accelerating Research through International Network-to-Network Collaborations
ACTRIS	Aerosol, Clouds, and Trace Gases Research Infrastructure
AI	artificial intelligence
AI4ESP	AI for Earth System Predictability
ALCF	Argonne Leadership Computing Facility
AMF	ARM Mobile Facility
AMIP	Atmospheric Model Intercomparison Project
AMP	AmeriFlux Management Project
API	Application Programming Interface
ARM	Atmospheric Radiation Measurement user facility
ARPA-E	Advanced Research Projects Agency-Energy
ASCR	DOE Advanced Scientific Computing Research program
ASR	Atmospheric System Research
BER	DOE Biological and Environmental Research program
BERAC	Biological and Environmental Research Advisory Committee
BES	DOE Basic Energy Sciences program
BESAC	Basic Energy Sciences Advisory Committee
BESC	BioEnergy Science Center
BETO	DOE Bioenergy Technologies Office
BGI	Beijing Genomics Institute
BRC	Bioenergy Research Center
BSL-3	biosafety level 3
BSSD	Biological Systems Science Division
CABBI	Center for Advanced Bioenergy and Bioproducts Innovation
CBI	Center for Bioenergy Innovation
CCSEM-EDX	computer-controlled scanning electron microscope with energy dispersive X-ray spectroscopy
CEDA	UK's Center for Environmental Data Analysis
CESM	NCAR Community Earth System Model
CMIP	Coupled Model Intercomparison Project
CO_2	carbon dioxide
COMPASS	Coastal Observations, Mechanisms, and Predictions Across Systems and Scales
COSORE	community database for continuous soil respiration
COVID-19	coronavirus disease 2019
CRAGE	chassis (or strain)-independent recombinase-assisted genome engineering
CRISPR	clustered regularly interspaced short palindromic repeats
CSP	Community Science Program
DEI	diversity, equity, and inclusion
DestinE	European Commission's Destination Earth
DFG	German Research Foundation
DKRZ	German Climate Computing Center
DoD	U.S. Department of Defense
DOE	U.S. Department of Energy
E3SM	Energy Exascale Earth System Model
ECMWF	European Centre for Medium Range Weather Forecasting
ECP	DOE Exascale Computing Project
ECRP	Early Career Research Program
ECS	equilibrium climate sensitivity
EERE	DOE Office of Energy Efficiency and Renewable Energy
EESM	Earth and Environmental Systems Modeling

EESSD	Earth and Environmental Systems Sciences Division
ELM	E3SM Land Model
EMSL	Environmental Molecular Sciences Laboratory
ENA	Eastern North Atlantic
ENIGMA	Ecosystems and Networks Integrated with Genes and Molecular Assemblies
ESGF	Earth System Grid Federation
ESM	Earth System Model
ESS	Environmental System Science
ESS-DIVE	Environmental System Science Data Infrastructure for a Virtual Ecosystem
EU	European Union
EUSAAR	European Supersites for Atmospheric Aerosol Research
FACE	Free-Air CO_2 Enrichment
FAIR	findable, accessible, interoperable, and reusable
FATES	Functionally Assembled Terrestrial Ecosystem Simulator
FICUS	Facilities Integrating Collaborations for User Science
FOA	funding opportunity announcemen
FY	fiscal year
FREDA	FT-MS R Exploratory Data Analysis
GCAM	Global Change Analysis Model
GCIMS	Global Change Intersectoral Modeling System
GFDL	NOAA Geophysical Fluid Dynamics Laboratory
GLBRC	Great Lakes Bioenergy Research Center
GSP	Genomic Science Program
HGP	Human Genome Project
IAM	integrated assessment modeling
ICON	Icosahedral Nonhydrostatic Weather and Climate Model
ICOS	Europe's Integrated Carbon Observation System
IDEAS	Interoperable Design of Extreme-scale Applications Software
IFL	Integrated Field Laboratory
ILAMB	International Land Model Benchmarking
IM_3	Integrated Multisector Multiscale Modeling
IMG/M	Integrated Microbial Genomics and Microbiomes
Input4MIPS	Input datasets for Model Intercomparison Projects
IPCC	Intergovernmental Panel on Climate Change
JBEI	Joint BioEnergy Institute
JGI	DOE Joint Genome Institute
KBase	DOE Systems Biology Knowledgebase
LDRD	laboratory-directed research and development
LTAR	Long-Term Agroecosystem Research Network
LTER	Long-Term Ecological Research Network
m-CAFEs	Microbial Community Analysis and Functional Evaluation in Soils
MIP	model intercomparison project
MKG	Microsoft Knowledge Graph
ML	machine learning
ModEx	model-experiment
MOSAiC	Multidisciplinary drifting Observatory for the Study of Arctic Climate
MS	mass spectrometry
nanoPOTS	nanodroplet processing in one-pot for trace samples
NASA	National Aeronautics and Space Administration
NASEM	National Academies of Sciences, Engineering, and Medicine
NCAR	National Center for Atmospheric Research
NEON	National Ecological Observatory Network
NERSC	National Energy Research Scientific Computing Center
NEXUS	Network for Execution of User Science
NGEE	Next-Generation Ecosystem Experiments

NICAM Nonhydrostatic ICosahedral Atmospheric Model
NIH National Institutes of Health
NMDC National Microbiome Data Collaborative
NOAA National Oceanic and Atmospheric Administration
NSA Northern Slope of Alaska
NSB National Science Board
NSF National Science Foundation
NSLS-II National Synchrotron Light Source II
NREL National Renewable Energy Laboratory
NVBL National Virtual Biotechnology Laboratory
OECD Organisation for Economic Co-operation and Development
OLCF Oak Ridge Leadership Computing Facility
ORNL Oak Ridge National Laboratory
PCMDI Program for Climate Model Diagnosis and Intercomparison
PFLOTRAN Parallel Reactive Flow and Transport model
PI principal investigator
PLpro papain-like protease
PMP PCMDI Metrics Package
PNNL Pacific Northwest National Laboratory
PuRe Public Reusable Research
QPSI Quantitative Plant Science Initiative
R&D research and development
RENEW Reaching a New Energy science Workforce
RFI Request For Information
SARS-CoV-2 severe acute respiratory syndrome coronavirus 2
SBIR Small Business Innovation Research
SciDAC Scientific Discovery Through Advanced Computing
SCREAM Simple Cloud-Resolving E3SM Atmosphere Model
SFA Science Focus Area
SGP Southern Great Plains
SPAC Special Purpose Acquisition Company
SPRUCE Spruce and Peatland Responses Under Changing Environments
STTR Small Business Technology Tra
TALENs transcription activator-like effector nucleases
TBS tethered balloon system
TEAMS Trial Ecosystems for the Advancement of Microbiome Science
TERRA Transportation Energy Resources from Renewable Agriculture
TMT tandem mass tag
TRACER Tracking Aerosol Convection Interactions Experiment
TRL Technology Readiness Level
UNESCO United Nations Educational, Scientific, and Cultural Organization
USDA U.S. Department of Agriculture
USGS United States Geological Survey
USQCD U.S. Lattice Quantum Chromodynamics computing project
VSV vesicular stomatitis virus
WCRP World Climate Research Programme
WDCC World Data Center for Climate
WGCM WCRP Working Group on Coupled Modelling
WHONDRS Worldwide Hydrobiogeochemical Observation Network for Dynamic River Systems
WoS Web of Science