BERAC Subcommittee on International Benchmarking: Findings and Recommendations

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Spring BERAC Meeting
April 22, 2022

Subcommittee

Many thanks to our support team!

- Tris West
- Wayne Kontur

- Mary Beth West
- Josh Nelson

- Holly Haun
- Marissa Mills

- Andrew Flatness

Charge letter questions to BERAC

- 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?

Report outline

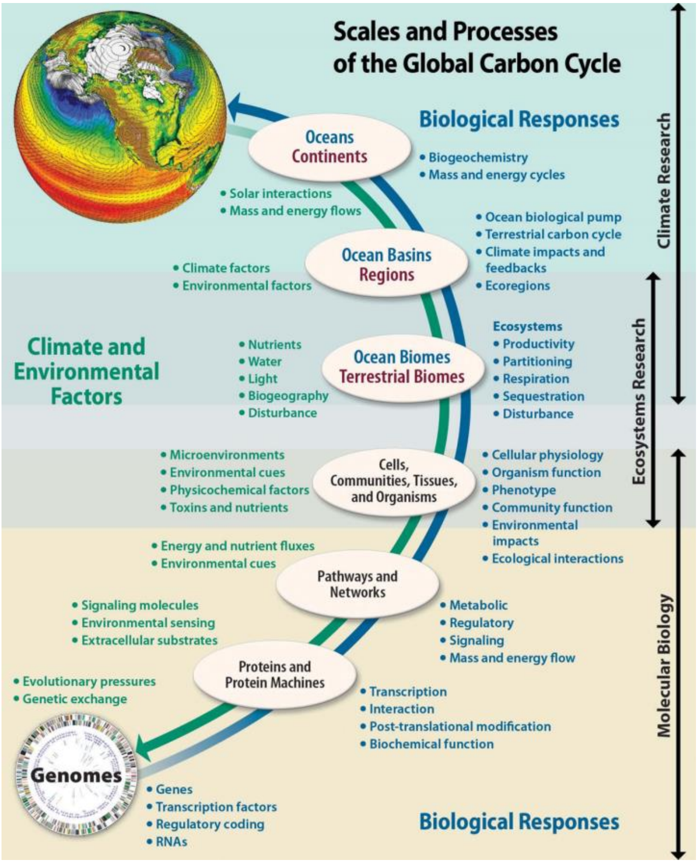
Executive summary

1. Introduction
2. Bioenergy and Environmental Microbiomes
3. Biosystems design
4. Environmental Science
5. Climate Science
6. Enabling Infrastructure
7. Integrative Science
8. Strategies for people, partnerships, and productivity

Reflections and Conclusions

Appendix A "Methodology"

Appendix B Abbreviations



General approach to metrics

Our goal is to benchmark performance in the last decade and to be generative for BER's strategy in the next decade with **actionable** recommendations.

- **Quantitative metrics** (e.g., bibliometric data, programmatic funding): used for benchmarking BER's practices, structures, protocols and resource investment, products and outcomes

- **Qualitative metrics** (e.g., responses to interview questions, Town Halls, public request for information): used for assessing the potential for international leadership in the next decade

Three important elements of the report: (1) BER products and their relative impacts as compared to other US and broader international programs; (2) compelling stories/case studies; and (3) a forward-looking perspective recommending opportunities to enhance BER's leadership over the next decade.

Presentation outline

- **Substantiated international leadership of BER**
- **Overarching findings**
- **Overarching recommendations**

  (Q and A, 10 mins)
- **Mission-specific recommendations and findings**

  (Q and A, 10 mins)
- **People, partnerships and productivity**
- **Reflections and conclusions**

  (Q and A, 10 mins)

Substantiated International Leadership of BER

BER-RELATED NOBEL PRIZE WINNERS

BER science is supported by a wide range of experimental, observational, and computational user facilities and services. These play an important role in the accomplishment of the BER mission, 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 IPCC 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 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. Looking 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 these mechanisms computationally.

2017
Joachim Frank

Nobel Prize in Chemistry

Awarded for the development of software used to reconstruct the three-dimensional (3D) structure of in situ biological molecules from transmission electron microscopy images. Frank, a NERSC user, pioneered the computational methods needed to reconstruct the 3D shape of biomolecules from thousands of 2D images obtained from Cryo-EM, methods employed today by most structural biologists who use electron microscopy.

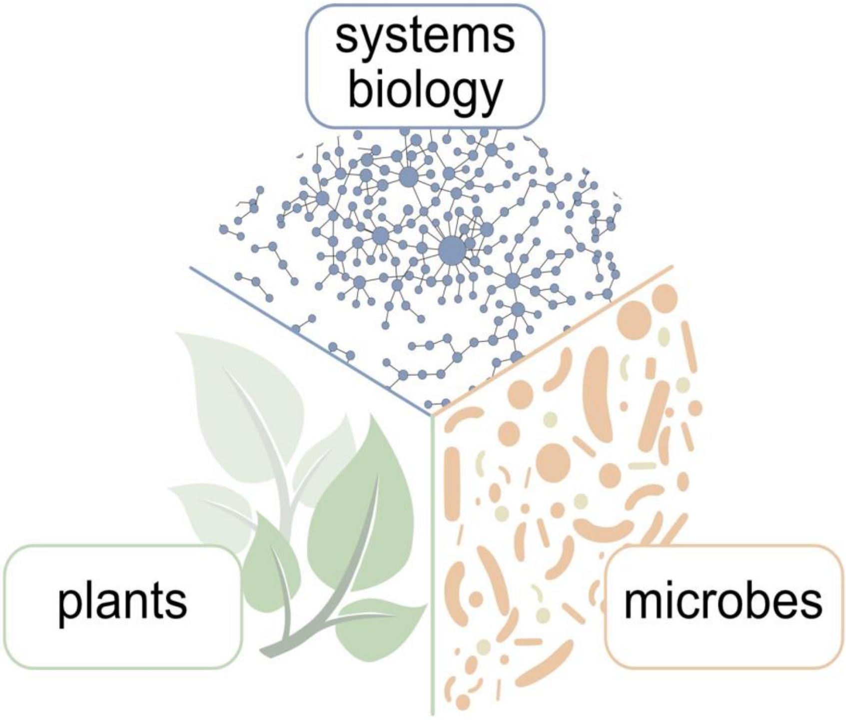
2020
- Jennifer Doudna
- Emmanuelle Charpentier

Nobel Prize in Chemistry

Awarded for for the "revolutionary impact on the life sciences' that their development of the CRISPR-Cas9 technology had." Doudna and Charpentier partnered with the Joint Genome Institute (JGI) to use the Integrated Microbial Genomics and Microbiomes (IMG/M) system to mine the immense collection of publicly accessible metagenomic data sets from a wide variety of ecosystems around the world, conducting iterative searches using statistical analyses to continuously refine and improve the process of finding novel Cas genes and CRISPR systems.

Bioenergy & Environmental Microbiome: Leadership Example

BER championed systems biology of bioenergy-relevant plants, microbes, and communities



Generation of genome-based resources - specifically in feedstocks - have had transformative impacts on bioenergy research, heralding innovations in predictive understanding and strategies to produce environmentally sustainable bioenergy

Long-term impact of DOE's leadership of this area:

Addressing climate change and national security concerns by providing the foundational knowledge needed for environmentally sustainable renewable energy and products for US's bioeconomy

Biosystems Design: Leadership Example

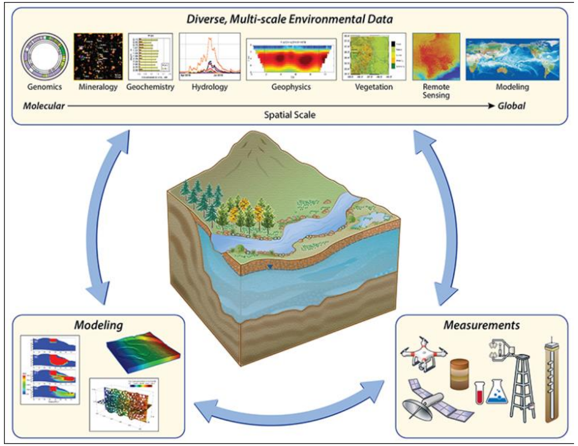
- In 2003, Amyris launched out of Jay Keasling's lab with a focus on artemisinin
- Pioneered yeast genetic engineering and fermentation technologies
- Saw huge potential for the technology to be applied to biofuels
- DOE funded Amyris to explore using US-based cellulosic feedstock
- DOE funding supported Amyris to build a pilot plant facility in Emeryville, CA
- Amyris' pilot plant is a critical differentiator and competitive advantage that enables Amyris to bring new products to market at unprecedented speed
- Amyris provides strategic counsel to DOE projects (e.g. JBEI/JGI), which play critical roles in the talent pipeline for Amyris and the entire biotech industry
- Has commercialized 13 fermentation-derived ingredients, found in >20,000 products, reaching >200 million consumers

Impact of BER's contribution:

Amyris has disrupted major markets and helped entire industries achieve sustainability with high-performing ingredients, at scale

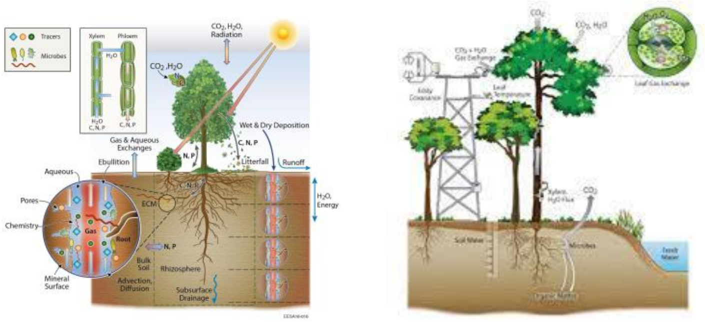
Environmental System Science: Leadership Example

Multi-disciplinary systems science



Data-Model Integration

Climate-ecosystem interactions across scales (NGEEs, AmeriFlux, Experiments, and Models)



Ecosystem-scale experiments and research infrastructure

Climate Science: Leadership Example

BER is an international leader through its PCMDI in climate model intercomparisons (including CMIP) and a leading contributor to IPCC assessment reports (ARs) and the 2007 Nobel Peace Prize to IPCC and Al Gore

- Larry Gates, the founder and former director of the DOE PCMDI, initiated the early AMIP and CMIP activities in 1989, which continues today - PCMDI led the AMIP1-2 and CMIP1-6 activities
- BER-supported researchers have been prominent in the IPCC assessment process, either as contributors, lead authors or coordinating lead authors, for all IPCC ARs (1990 - 2021).
- LLNL/PCMDI led the innovative Earth System Grid Federation (ESGF) development, building a global federation for petabyte-scale data access, and continues to develop the PCMDI Metrics Package (PMP) for comprehensive Earth system model evaluation

PCMDI CMIP leadership has empowered the global climate research community, and this continuing project has advanced climate understanding and underpinned global climate policy decision-making.

Enabling Infrastructure: Leadership Example

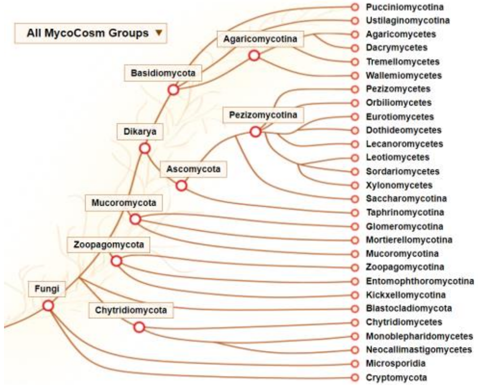
Joint Genome Institute @ 25

- The long running, largest genomic science center worldwide exclusively performing DOE mission-relevant (non-biomedical) genomics research.
- Offers unique access to large-scale data production and cutting-edge capabilities to a global community of users.
- JGI's MycoCosm targets large-scale sequencing and analysis of fungal genomes to explore the phylogenetic and ecological diversity of fungi, and integrates fungal genomics data and analytical tools, promoting user community participation in data submission, annotation and analysis.

JGI @ 25: Fruiting bodies of *Laccaria bicolor* colonizing seedlings of Douglas fir. (Francis Martin).

Impact

- 2016. JGI capabilities enabled environmental metagenomics to provide unprecedented insight into the composition and functioning of whole microbial communities controlling the cycling of carbon and nutrients in the environment. Thousands of complete microbial genomes were recovered through terabase-scale (10^{12} DNA bases), cultivation-independent metagenomic sequencing of an aquifer sediments community.
- 2017. Researchers using the JGI user facility successfully adapted a yeast DNA recombination system to engineer the entire pathway of a soil bacterial pigment into a plant, as well as to drop in an entire biodiesel metabolic pathway. By radically simplifying stacking of genes from different sources and engineering them into a different organism, the work is a significant advance toward developing new biotechnology tools for use in a broad range of plants.



JGI's MycoCosm search form

Enabling Infrastructure Case Study: COVID-19 #NatLabsInTheFight

NVBL

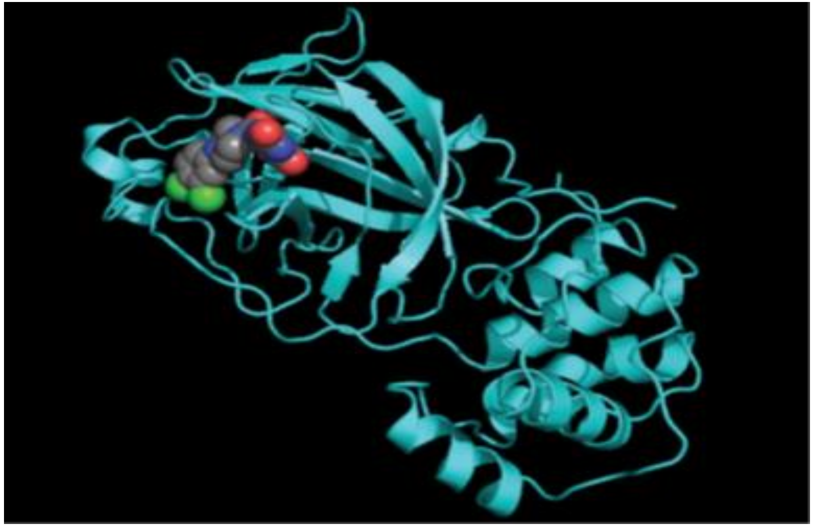
- DOE established the NVBL in 2020 under BER leadership, bringing together scientists from across the DOE Laboratory system and utilizing **DOE light and neutron sources, cryogenic electron microscopy (cryo-EM), cryo-tomography, and the DOE LCFs**.

Molecular Design of Covid-19 Therapeutics

- DOE capabilities in HPC and AI combined with the structural biology, chemistry, and analytical capabilities of the national laboratories were applied to accelerate discovery of small molecules and antibodies that interact with key viral targets.

Antibody Discovery

- By modifying three existing antibody scaffolds known from prior SARS outbreaks, create new antibodies to bind and neutralize SARS-CoV-2.
- AI was used to sample more than 10^{40} possible antibody variations, enabling down-selection to 300 designed antibodies.
- Experimental screens confirmed hits for all three antibody scaffolds. Optimization is on-going.



Inhibitors of Viral Cysteine Proteases

- Viral proteases 3CLpro and PLpro that are not amenable to traditional drug discovery methods were targeted
- Tens of millions of small molecules were computationally screened against more than 100 binding sites of the SARS-CoV-2 viral proteins resulting in down-selection of 2000 small molecules.
- Experimental validation was performed at **DOE BES light sources using beamlines co-funded by BER**.
- Antiviral screening showed that 56 molecules inhibit viral infection in the cell-based assay. Discovered a potent PLpro inhibitor that rivals remdesivir.

World-leading capability

- Therapeutic discovery effort would not have been possible without close integration

No other organization in the world had the capability to screen so many possible targets

Case Studies

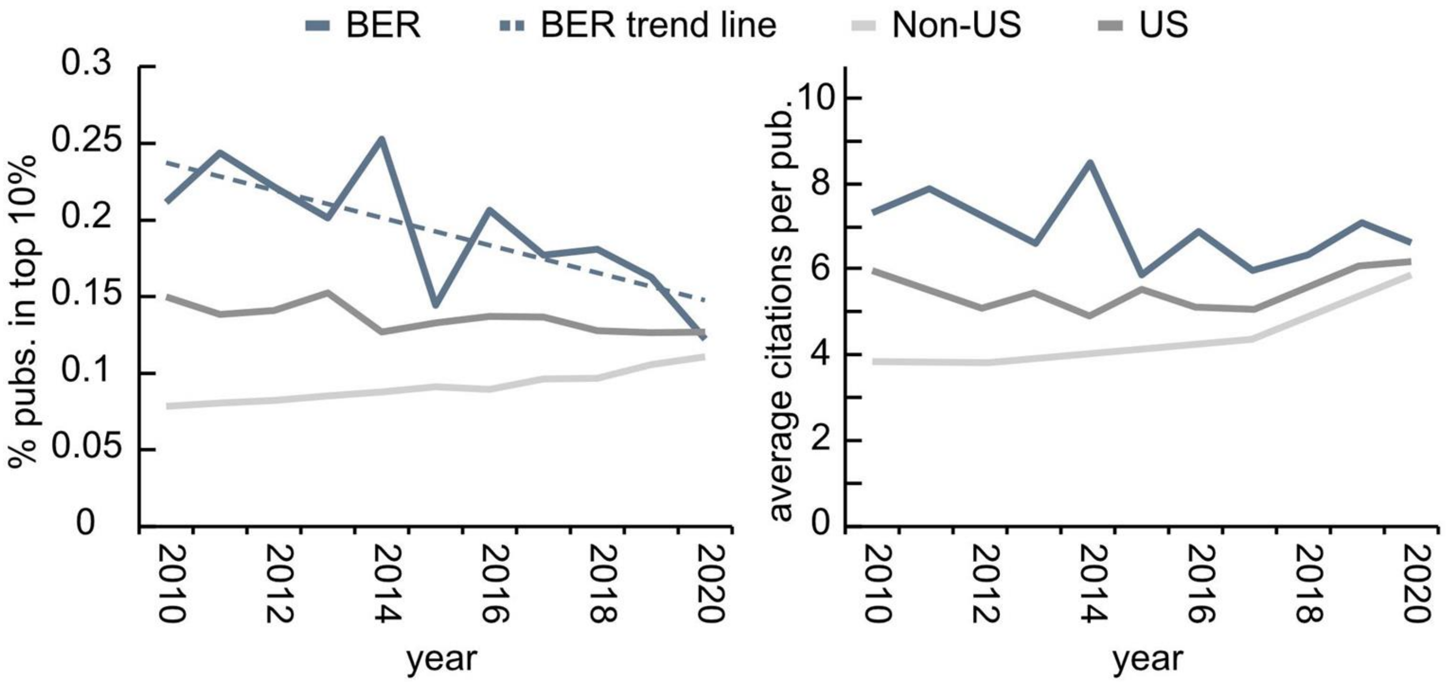
Title	Mission area	Benchmarking message
The Bioenergy Research Centers	Bioenergy and Environmental Microbiomes	Well-managed, mission-inspired, scientific Centers can be successful and sustained collaborative funding can increase impact
Ginkgo	Biosystems Design	DOE-funded workforce training before PhD level is essential for the future bioeconomy
Amyris	Biosystems Design	Supported in-part by DOE, Amyris has disrupted major markets and helped entire industries achieve sustainability with high-performing ingredients, at scale
Next-generation ecosystem experiments: Tropics and Arctic	Environmental Systems Science	Explicit connection of scientific understanding of these ecosystems to the Exascale Earth System Model is a paradigm shift
Interoperable Design of Extreme-scale Application Software (IDEAS)	Environmental Systems Science	A community approach has enabled leadership in computational modeling of ecosystems with high process fidelity at a variety of spatial scales
Coupled Model Intercomparison Project (CMIP)	Climate Science	DOE support of, and leadership in, CMIP has been vital for its far-reaching success in the international climate science community
Cloud feedbacks and climate sensitivity	Climate Science	DOE is a world leader in understanding how clouds affect Earth’s energy budget, how and why cloud properties change under climate change, and Earth’s sensitivity to carbon dioxide
COVID-19 #NatLabsInTheFight	Enabling Infrastructure	An enabling infrastructure coupled to diverse capabilities can be entrained for a rapid and impactful national response
Horizon Europe and Destination Earth	Integrative Science	New European investments are improving integration of climate, ecosystem and impacts science

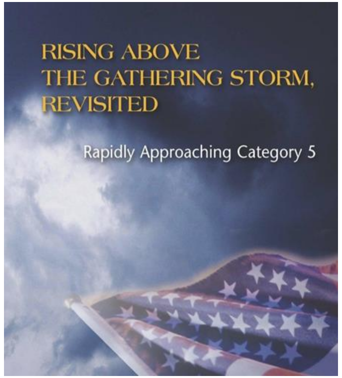
Overarching Findings & Recommendations

Overarching Findings

- BER’s international leadership is well-substantiated across mission areas and enabling infrastructure
- BER’s mission areas are increasingly recognized as the critical challenges for the coming decades, for which big science can and must be entrained
- “International leadership” need not be adversarial – leadership in a collaborative context is viewed as a more meaningful goal
- Future leadership is not guaranteed and will require increased investments and strategic partnerships (private-public-academic, intra- and inter-agency, international, and across disciplines)
- Volatility in priorities, funding, and workforce retention poses a significant threat to BER’s ability to sustain its leadership
- The last decade of funding support did not grow in contrast to the scale and growing acuteness of the national and global challenges addressed by BER
- Major research impacts and achievements are not widely recognized as associated with BER

Predictions from the “Gathering storm” report might now be showing up in publication and citation trends



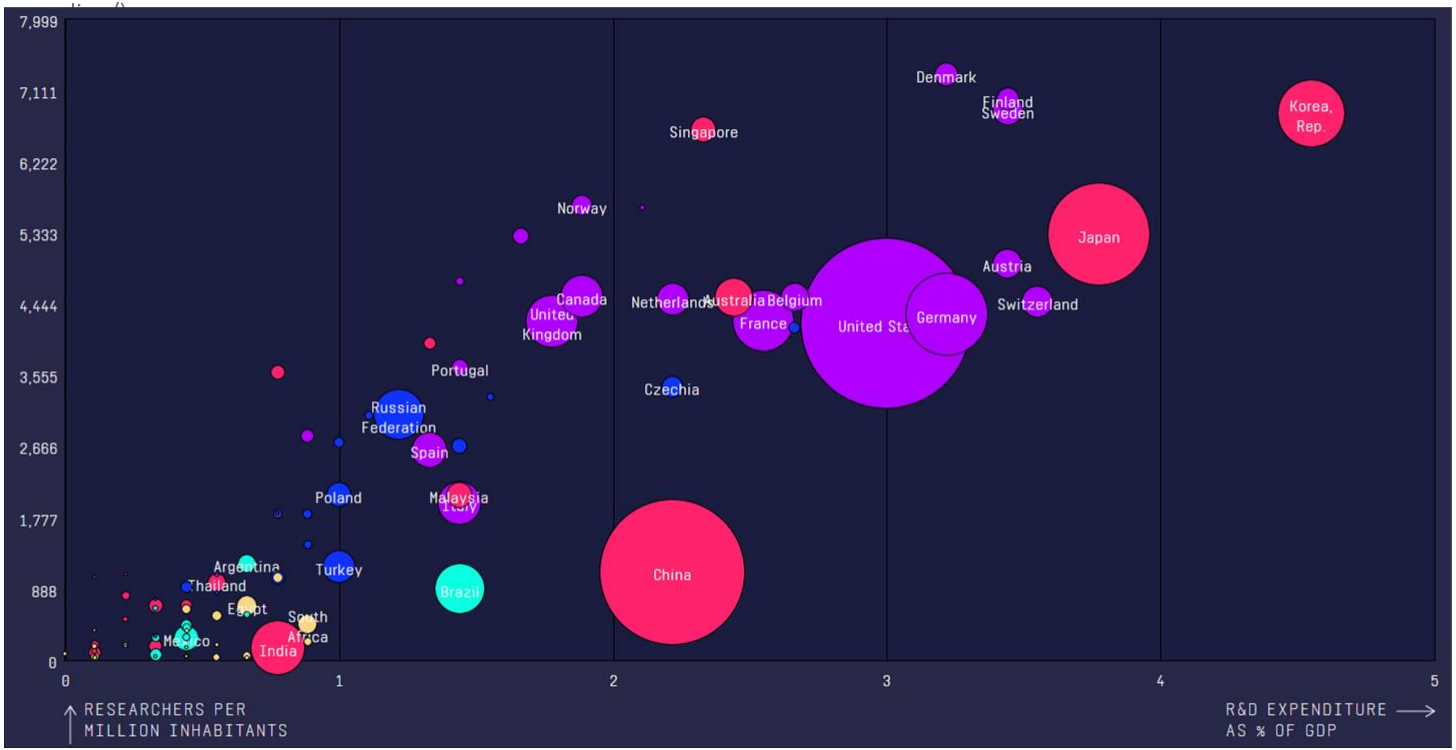


NASEM Press, 2010

Comparison groups are BER, domestic, and non-domestic. Relative representation ratios are (% representation in bracket) / (% representation in total publications).

International Research Funding Context

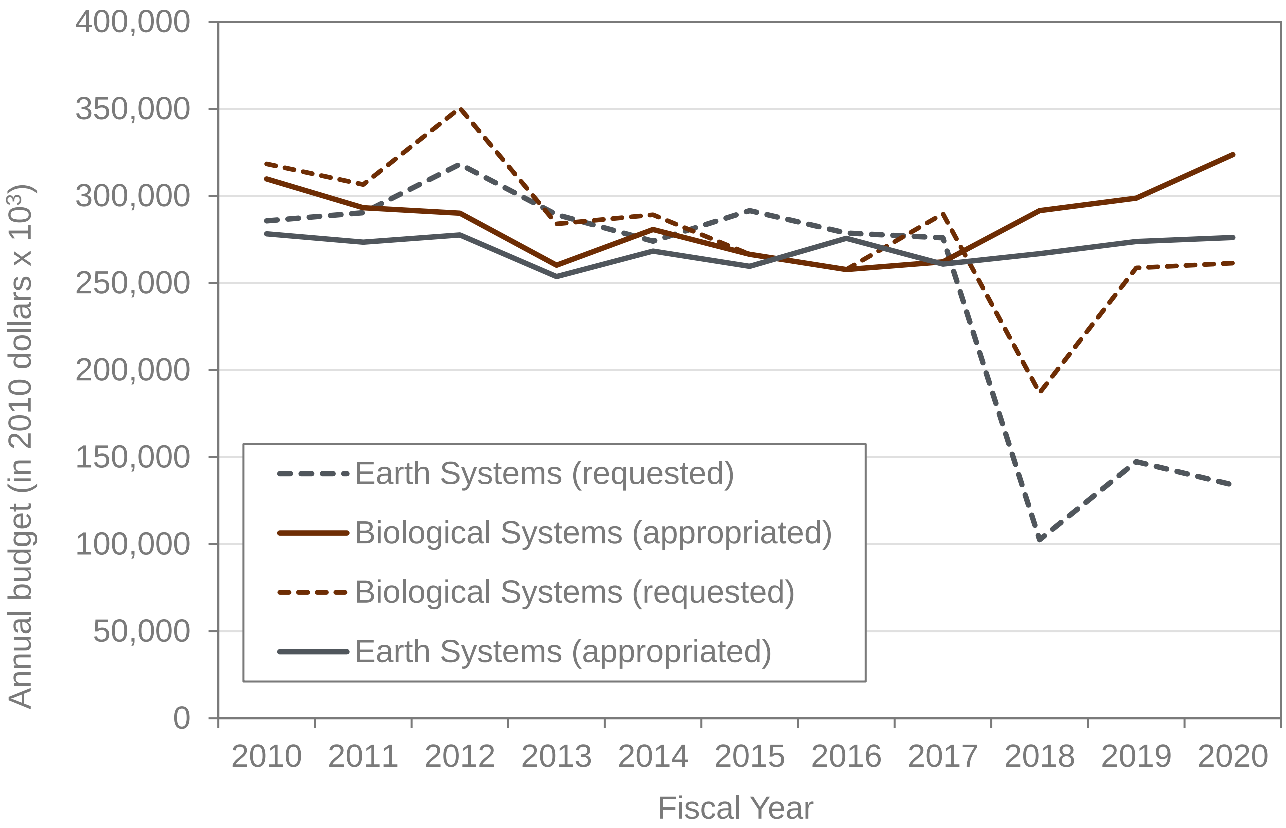
UNESCO Institute for Statistics notes over the last decade Global R&D has increased to record levels (~$2-Trillion as of 2019) with countries pledging substantial increases in public and private funds as well as the number of researchers by 2030 as part of their responses to the Sustainable Development Goals. (http://uis.unesco.org/apps/visualisations/research-and-development-



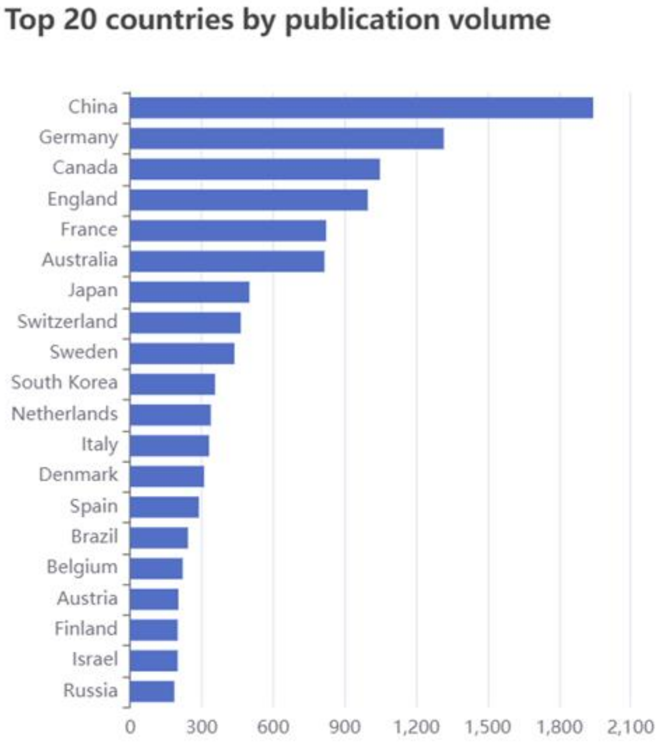
Circle Size = Purchasing Power Parity Dollars Spent

US R&D as % GDP risks falling out of top 10 globally

Volatility threatens BER’s international leadership



Ranking of countries with collaborative co-authorship in BER publications (2010 – 2020)



Joint publications with international co-authors are highly cited

Overarching Recommendations

- Increase and sustain resources needed in all mission areas and integrative science across and between mission areas (risk: failure to invest)
- Better connect basic science to research across technology readiness levels (risk: failure to capitalize on investment)
- Put horizon scanning mechanisms in place 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, early- and mid-career professional development, and delivers the future workforce (risk: failure to sustain future leadership)

Bioenergy & Environmental Microbiome: Findings & Recommendations

Bioenergy & Environmental Microbiome: Findings

BER is an international leader in

- fundamental bioenergy sciences, sustainability, and environmental microbiomes
- developing/applying genome-based and omics approaches to bioenergy research and in environmental microbiomes
- plant bioenergy and feedstock research

The next frontier will be the application of multi-omics combined with additional technologies, including innovative advancements in microbial and plant biochemistry, where BER may be lagging behind some other countries.

Some other countries are seen as better at the deployment of applications and translation to marketable products.

The BRC program exemplifies the power of well-managed team science that has benefitted from stable funding, a strong mission, and emphasis on collaboration.

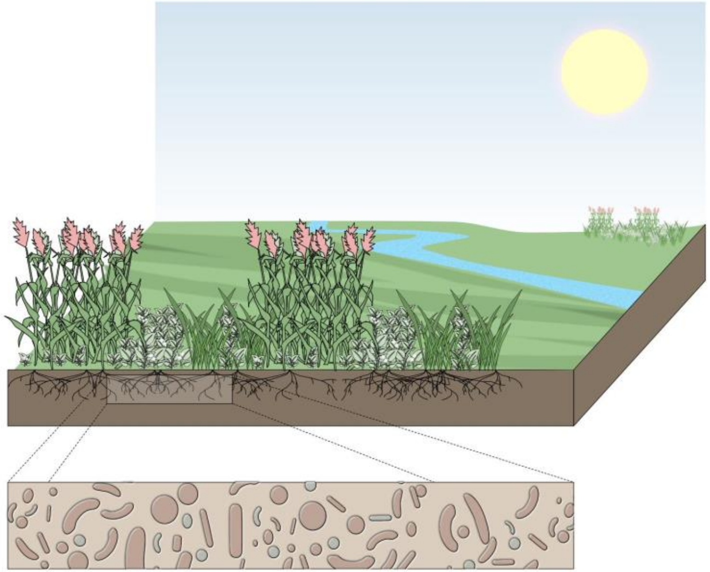
Bioenergy & Environmental Microbiome: Recommendations

- To maintain international leadership, BER should support and encourage the next-generation of researchers to launch a revitalization in bioenergy that embraces innovative, high-risk approaches.
- BER should seek a leadership role in providing the fundamental knowledge needed to bring products to market by building bridges between early Technology Readiness Levels (TRLs).
- Enable interactions and inter-disciplinary collaborations that better integrate knowledge between and across experimental scales, from computation-to-experimentation and molecules-to-phenotypes and provide access to established resources (such as field experiments).
- Build on internationally recognized strengths and leadership in genome-enabled knowledge in bioenergy and environmental microbiome research areas to understand the complex interactions between bioenergy crops and environmental microbiomes that will provide the foundation for management of ecosystem sustainability in the face of a changing environment.

Bioenergy & Environmental Microbiome: Recommendation example

Build on internationally recognized strengths and leadership in genome-enabled knowledge in bioenergy and environmental microbiome research areas to understand the complex interactions between bioenergy crops and environmental microbiomes.

- The BER research portfolio has the people and tools needed to form large-scale research teams who in partnership can build a holistic, multi-scale, predictive understanding of sustainable bioenergy cropping systems, their microbial communities, soil health, and ecosystem-level processes.



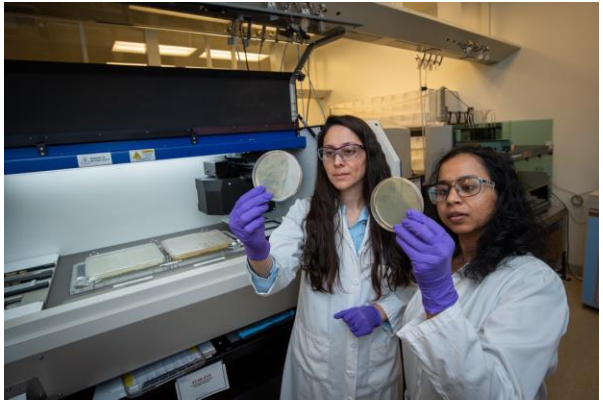
Leveraging systems biology approaches to gain predictive understanding of above- with below-ground communities for an environmentally sustainable bioeconomy

Outcome:
Management of ecosystem sustainability for an environmentally sustainable bioeconomy in the face of a changing climate.

Biosystems design: Findings & Recommendations

Biosystems Design: Findings

- BER's launch of Biosystems Design (BSD) research is relatively new, but is off to a strong start.
- BSD has a strong overlap with Bioenergy in the BER portfolio, with many of these efforts being high-profile.
- The US/BER is considered to have a strong leadership position in microbial biosystems design, but this leadership is increasingly distributed across the globe.
- Particular strengths are noted in bacterial systems, while the US is considered "one of many" for yeast and other fungi.
- The US/BER is not viewed as leading with respect to understanding microbial physiology during scale-up.
- No region was viewed as leading with respect to plant biosystems design, suggesting that this is an area where targeted investments could yield substantial intellectual returns.



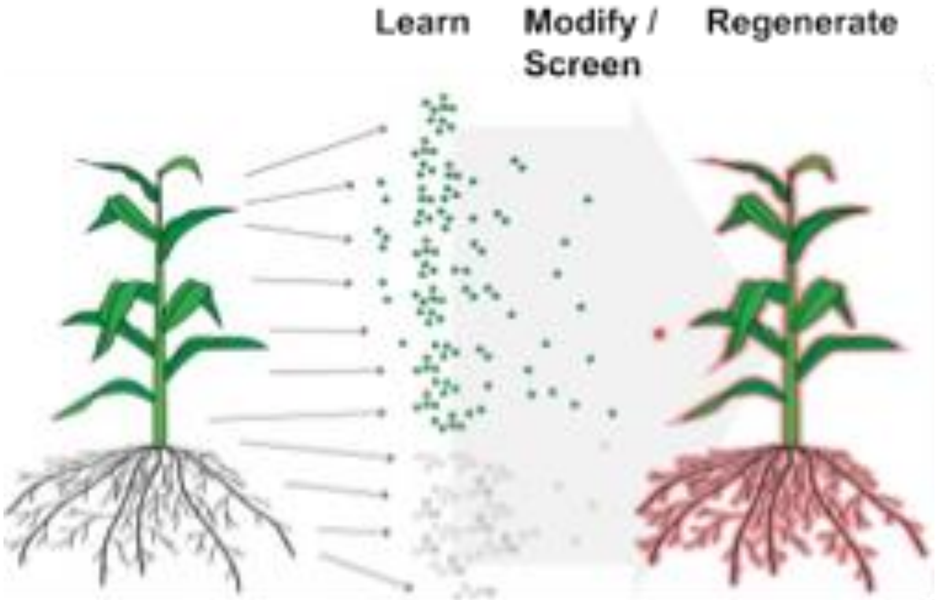
Biosystems Design: Recommendations

1. Establish new BRC-like Biodesign Research Centers
2. Coordination of joint funding calls with international funding agencies to accelerate the pace of progress in biodesign by leveraging key expertise found in different countries
3. Attempt to replicate the recent breakthroughs of machine learning (ML), e.g., using AlphaFold2.0 for protein folding, in biodesign. Targeted funding for curating, mining and generating omics datasets that can be used to train ML models to support biodesign
4. Addition of a bioenergy research center that leverages non-model microbes including photosynthetic microbes for biofuels, biorenewables and materials production
5. Invest in disruptive, bold initiatives to accelerate processes of plant transformation
6. BER BSSD should grow its support for biomanufacturing projects that train the PhD and non-PhD workforces that play critical roles in the talent pipeline for the entire U.S. biotech industry

Biosystems design: recommendation example

Invest in disruptive, bold initiatives to accelerate processes of plant transformation

- DNA delivery
- Tissue regeneration
- Increased throughput
- Genotype independence
- Genome editing
- Prevention of gene flow



Outcome:
Accelerate innovation cycles for bioenergy crop species

Image from Jennifer Brophy

Silva et al, (2020) J. Expt. Botany

Environmental Systems Science: Findings & Recommendations

Environmental Systems Science: Findings

ESS research is very well cited and internationally respected for:

- Multi-disciplinary, systems science
- ModEx, iteration of models and experiments leading to novel discoveries
- Research infrastructure, such as SPRUCE, AmeriFlux, and Watershed “collaboratories”
- Terrestrial Ecology: biogeochemistry, ecosystem fluxes, and climate change responses.
- Watershed Sciences: multi-scale hydro-bio- geochemical modeling and process studies

ESS research has untapped potential for:

- Better integration of human influence in the study of natural systems
- Creative discovery science, yet also translating research to inform applied solutions
- Bridging the gap between terrestrial sciences and atmospheric and modeling sciences

Environmental Systems Science: Recommendations

- Invest at the intersection of human-natural systems, to stay on the leading edge of fundamental ESS science in a changing world.
- Elevate and integrate tools for data discovery and analysis commensurate with the data complexity produced by ESS BER, to accelerate scientific impact and value to models.
- Facilitate translation of ESS research to innovation and solutions. Create avenues for communication and interaction across the DOE S&T pipeline, to inspire breakthroughs and to reduce institutional barriers, time lags, and the need to reinvent the wheel.
- Make BER ESS an international leader in safe and inclusive fieldwork, anchored on its existing accomplishments, to help build and model equitable professional environment.
- Maintain leadership in pioneering ecosystem manipulation experiments, a hallmark of BER, to integrate ESS, promote ModEX, and foster collaboration among institutions.
- Expand the paradigm for ESS strategic goals and funding–for more process-based discovery and exploratory research–to ensure continued international domain leadership.

Environmental Systems Science: Recommendation Example

Invest at the intersection of human-natural systems, as a niche for BER ESS contributions, in the coming decade

- The impacts of humans are ubiquitous, in climate, hydrologic, and elemental cycles.
- This is a frontier in ESS, yet BER is only beginning to study direct (e.g., urban landscapes) and indirect roles of humans (e.g., water diversions)
- Fundamental research on environmental systems in the context of human influence will enhance discovery and predictive capabilities
- Capacity for leading in this area is evident in e.g., new Urban Integrated Field Laboratories, Coastal Systems opportunities, and NGEE and SFA funding modes

<u>Desired outcome:</u>

- BER maintains leading edge of fundamental ESS science in a changing world, and its science informs use-inspired innovation and solutions to pressing problems.

Climate Science: Findings & Recommendations

Climate Science: Findings

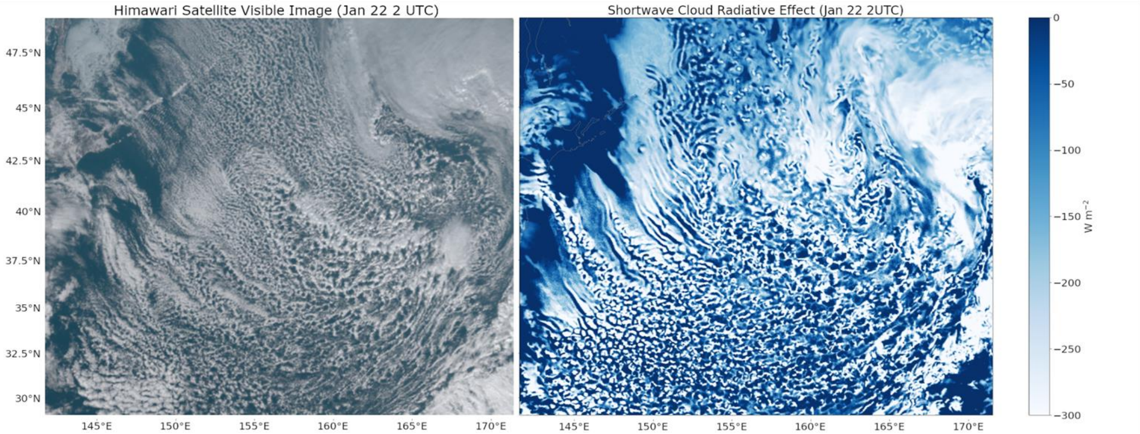
- BER-funded climate science publications are cited on average more often than other publications, particularly for top 1% and 5% of most cited publications.
- BER has been an international leader in climate model intercomparisons (AMIP/CMIP) through PCMDI and a leading contributor to the 2007 Nobel Peace Prize awarded to the IPCC and Al Gore.
- BER is a world leader in studying climate change and cloud feedback. Its climate research has a close connection to the 2021 Nobel Prize Winner in Physics – Syukuro Manabe and Klaus Hasselmann.
- BER is one of a few world leaders in developing kilometer-scale Earth System Models by advancing exascale computing (E3SM). Germany and Japan are competitors.
- BER is perceived as a natural home for developing capabilities in cross-cutting energy-related research and coupled human-Earth systems (e.g., GCAM).
- BER is a clear leader internationally in ground-based and aerial measurements (ARM) and their use to advance physical understanding of atmospheric systems (ASR).

Climate Science: Recommendations

- Maintain leadership in US development of kilometer-scale Earth system model by advancing exascale computing, using AI/ML approaches, and integrating observations
- Maintain international leadership in coupled human-Earth system modeling and provide more decision-relevant insights
- Maintain international leadership in ground-based and aerial measurements and their use to advance physical understanding of atmospheric systems, strengthen collaborations with satellite community and integration of national and international field observing systems
- Maintain international leadership in cloud feedback and climate model intercomparison through increased support of PCMDI and ESGF
- Seek to establish sustained and substantial funding streams to support expanded collaboration with US agencies and universities, and also create additional means for supporting blue sky proposals from DOE scientists to stimulate innovation and workforce engagement

Climate Science: recommendation example

- Continue to lead the US development of kilometer-scale Earth system modeling (ESM) by advancing exascale computing, use of AI/ML approaches, and model-observation integration



DOE E3SM Storm-Resolving Model (SCREAM) Simulation of Cold-air outbreak off Siberia. Satellite Image (left) and SCREAM Simulation (right)

- The initial success of the E3SM 3-km convection permitting model has put BER in a position of leading the U.S. contributions and joining a few world leaders in this field in the future
- The kilometer-scale ESM is key for properly simulating critical Earth system processes and extremes and strongly motivates the integration of cutting-edge computational technologies and climate science for actionable projections of future climate changes.

Enabling Infrastructure: Findings & Recommendations

Enabling Infrastructure: Findings

BER capabilities are world-leading:

Joint Genome Institute. JGI is the largest genomic science center worldwide exclusively performing DOE mission-relevant (non-biomedical) genomics research.

National Synchrotron Light Source II (NSLS-II). NSLS-II is the U.S.'s newest and most advanced synchrotron. The design optimizes the creation of tightly collimated, high flux light beams, covering the spectral range from infrared to high energy x-rays.

Atmospheric Radiation Measurement. ARM is internationally recognized for its long-term ground-based observations facilities, which have been advancing atmospheric and climate research globally for 40 years.

ASCR Leadership Computing Facilities. ALCF, OLCF, and NERSC form the ASCR Leadership Computing Facilities (LCFs) and are a critical part of the enabling infrastructure that BER scientists rely on. In November 2021, OLCF's Summit system placed second, and NERSC's Perlmutter system was ranked fifth in an international benchmarking by the High Performance Computing (HPC) community.

AmeriFlux/AmeriFlux Management Project (AMP). AmeriFlux is one of two leading flux networks in the world and is an essential contributor to the global flux network. It is part of the international FLUXNET and has taken the lead in creating the FLUXNET synthesis data products, the most impactful international observational product.

Enabling Infrastructure: Recommendations

- Create an oversight board that assesses strategic decisions regarding the creation, continuation, and sunsetting of infrastructure capabilities across the full BER infrastructure portfolio. This board should develop and publish a regularly updated roadmap for future infrastructure capabilities that optimally supports the mission-critical science focus areas. The capability strategy and roadmap should be coordinated with other relevant DOE offices and peer national and international agencies to maximize investment and impact.

- Promote greater integration across facilities that enables users to easily schedule and use different infrastructure capabilities, including support for integrated data management and analysis.

- Consider the creation of data user facilities to provide long-term governance, planning, policy development, modern technology, and support for this critical type of enabling infrastructure.

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

- Increase provision of computational and storage capacity for BER researchers.

Enabling Infrastructure: Recommendation Example

Create a diverse oversight board that assesses strategic decisions regarding the creation, continuation, and sunsetting of infrastructure capabilities across the full BER infrastructure portfolio. This board should develop and publish a regularly updated roadmap for future infrastructure capabilities that optimally supports the mission-critical science focus areas. The capability strategy and roadmap should be coordinated with other relevant DOE offices and peer national and international agencies to maximize investment and impact.

- BER's enabling infrastructure capabilities currently operate as an independent collection of DOE user facilities and project-based services.
- Some collaboration among biological systems science resources, such as JGI, EMSL, and NSLS-II on an operational basis.
- It is not clear if a long-term roadmap exists for BER capability development
- Not clear if there are strategic joint planning activities with other DOE offices or agencies to identify opportunities for collaborative or synergistic infrastructure development.
- There are world-leading capabilities, e.g., JGI and ARM, but their leadership positions are under threat by strategic facility developments worldwide, where integrated, long-term planning models exist.
- The recent NVBL effort highlighted the benefits of an integrated set of capabilities, spanning from computing and data to leading experimental facilities.

Integrative science: Findings & Recommendations

Integrative science: Findings

- ARM and ASR are international leaders of integrative science around short-term field campaigns
- BER is relatively ahead internationally in the integration of climate observations and modeling
- Maintaining ARM/ASR and ESM/observation integration leadership will depend on staying up to date observationally and continued access to adequate computational resources (a possible concern)
- Much is yet to be gained from improving integration across E3SM, PCMDI, ARM and MSD efforts
- Integrating efforts across US agencies is a formidable challenge, leaving unrealized opportunities; (The EU is pursuing a centralized modeling program in part to address that - see DestinE case study)
- The Bioenergy Research Centers are exemplary loci of interdisciplinary research, ranging from ecosystem modeling to detailed molecular analysis.
- EMSL and JGI, along with their numerous collaborators, are hubs for integration (MOSAIC and FICUS as examples) and international leaders in ‘omics research, molecular and structural analysis, and systems biology.
- EMSL successfully integrates atmospheric science and physical chemistry, with the potential for expansion into the area of biological aerosols.
- BER research leads in obtaining systems level understanding - particularly in microbiome and ecosystem function.
- BER beamlines at DOE Light Sources provide world-leading capabilities and are leaders in structure determination.
- 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.

Integrative science: Recommendations

Improve BER's capacity for multidisciplinary integrative research

- Create programs that cross BER Divisions, DOE, and, where possible, other agencies that leverage BER research strengths and advance BER's research agenda
- Establish long-term field sites as platforms for integrated empirical studies that span genomes-to-landscapes and subsurface-to-atmosphere, with associated computational capacities
- Explicitly include coupled human-natural system dynamics in funding opportunities across BER
- Establish a synthesis and integration user facility with computational, visualization, and training resources that supports research that demands targeted integration across disciplines and scales

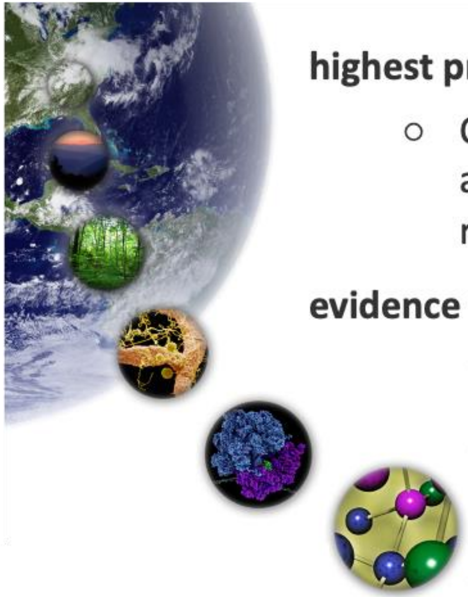
Better integrate BER's existing and future efforts in climate change forecasting and decision making

- Work with other US agencies to establish a joint effort to deliver state-of-the-art climate and environmental data forecasts from a centralized national platform in the formats needed by stakeholders
- Establish a multi-agency research program in coupled human and earth systems analysis to improve integration across both domestic and international programs

Long-term impact of DOE's leadership of this area

- A vibrant and multidisciplinary scientific community, where all researchers work across disciplinary lines to advance BER research for the coming decades
- Multi-dimensional scaling is a grand challenge area, and demands interdisciplinary collaboration
- Translation of fundamental science to the applied domain will speed the process of solving grand challenges

Integrative science: recommendation example



highest priority recommendation:

- Create cross-program, cross-DOE, cross-laboratory, and, where possible, cross-agency funding opportunities that leverage expertise and capabilities across the range of unique BER research strengths

evidence that supports the recommendation:

- few opportunities for BSS-funded scientists to meaningfully participate in place-based projects led by ESS
- too few opportunities to connect genome-level organismal science with biogeochemical and process-based research
- e.g. in NGEE program, proposals with too-strong a genomic focus were not prioritized
- few opportunities for ESS-funded scientists to meaningfully participate in BSS-led bioenergy programs
- analysis of FICUS (JGI-EMSL) found little evidence of cross-Division projects

desired outcome:

A vibrant and more interconnected scientific community, where all researchers have freedom to work across disciplinary lines, will provide the foundation for cutting-edge BER research for the coming decades

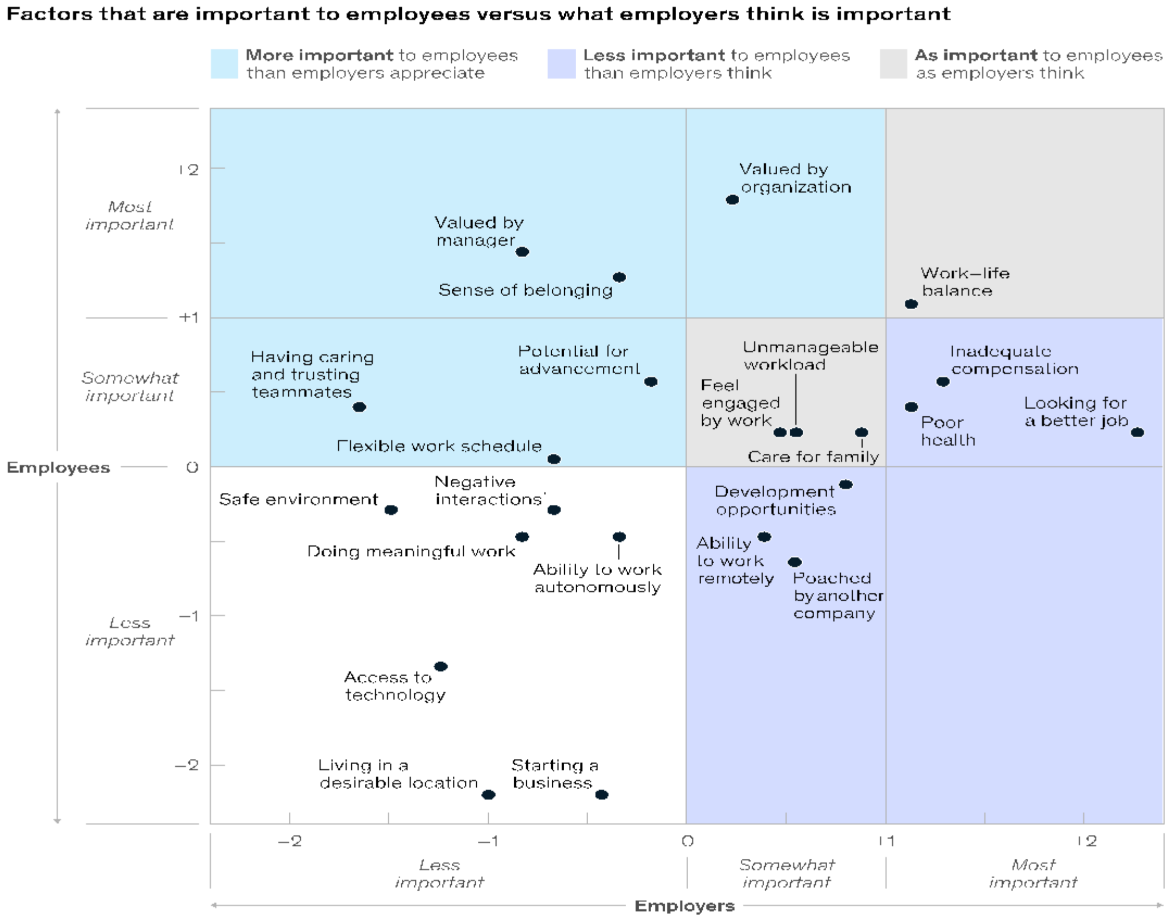
People, Partnerships, and Productivity Findings & Recommendations

People: Findings

Leadership is….."producing the next generation of scientists"

- Academic scientists funded in BER mission space bring exceptional talent, contribute new expertise, and enable participation in all 50 States.
- In the National Lab complex, there are many positive aspects for careers
- Summer Schools and Programs for undergraduate, graduate students and post-docs are effective recruiting tools to BER mission space
- Lack of workforce diversity is an issue for the talent pipeline
- Volatility and perceived volatility in funding levels and in FOA topics create challenges for recruitment and retention at all career stages, and for long-term productivity
- Anxiety is created in the National Lab context because of the model of staff having to find projects that support their own salaries
- Funding support for blue sky research and paths to independent work are rare in the National Lab context and increased funding flexibility is desired at all career levels
- There is lack of visibility of BER research frontier successes and impacts

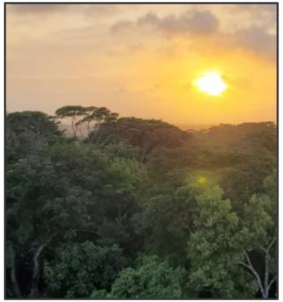
People

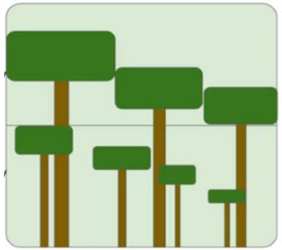


In the future of work, employers might attract and retain employees by focusing on relational, not transactional, aspects of their culture.

De Smet, Dowling, Mugayar-Baldocchi, Shanninger "Great attrition or great attraction – the choice is yours" McKinsey Quarterly, September 2021

ESS Case Study: Next Generation Ecosystem Experiments (NGEE)





- The NGEE projects bring together multi-disciplinary, multi-institutional teams to support both discovery science *and* integration of knowledge into DOE's Energy Exascale Earth System Model (E3SM).
- They have flagship science accomplishments, such as the development of the trait-based, ecosystem demography model FATES, integrated in E3SM.

- They also have flagship accomplishments for people and partnerships. The size and length of these investments has allowed them to:
  – Execute intentional steps to improve DEI in BER research, such as building cultures of safety and inclusion, operating under exemplary codes of conduct, and hosting bystander trainings.
  – Build team culture, such as mentoring rising leaders, advancing data sharing, and executing on succession plans.
  – Integrate effective international and multi-agency partnerships into the research activities, governance, and domain leadership

People: Recommendations

- Incentivize efforts to increase workforce diversity and promote a culture of inclusivity
- Better support BER early-career award researchers for their future, post-award, career path
- Incentivize the national laboratories to create professional development opportunities for early and mid-level career scientists
- Models of collaborative teaming paths vs individual successes need to be developed and demonstrated
- BER should take a proactive approach in communicating its research mission to recruit and retain top global talent

Partnerships: Findings

"International competitiveness"?........leadership in "an international, collaborative context" is the meaningful goal

- International collaboration is critical for strengthening BER science output and increasing global visibility. However, it is currently difficult for the BER-funded institutions to collaborate with international partners due to funding restrictions between countries.
- BER program staff have few resources to travel and engage internationally
- There is a need for more collaboration domestically and internationally in the areas from ground-based observations to high-resolution Earth system modeling to improve research outcomes and ensure integration of efforts to meet societal needs.
- ARM's partnerships internationally (such as the Polarstern cruises during MOSAiC) and domestically (such as the TRACER campaign with NASA and NSF) are highly successful, which is enabled by the ARM Mobile Facilities and the ability to fund international partners

Partnerships

"S&E is now a truly worldwide enterprise, with more players and opportunities, from which humanity's collective knowledge is growing rapidly."

NSB Vision 2030 report

NATIONAL SCIENCE BOARD

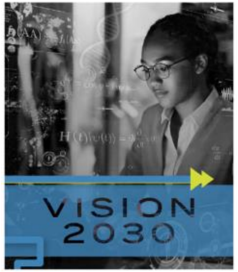
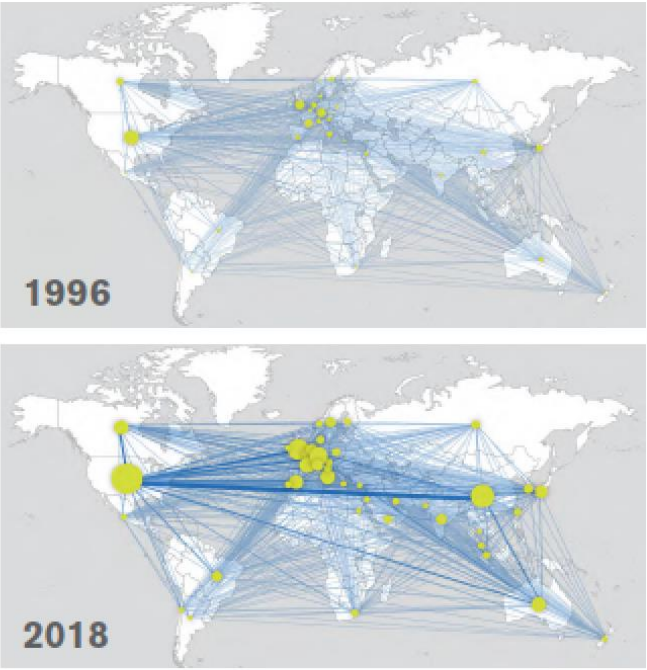


FIGURE 4: INTERNATIONAL COLLABORATION AMONG RESEARCHERS GROWS DRAMATICALLY



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 have grown – as shown by the width of the lines, with the size of the circles denoting the relative number of publications. Now, China has emerged as the single most frequent partner with the U.S. in research collaboration.

Source: NSB, "Publications Output: U.S. Trends and International Comparisons," *Science & Engineering Indicators 2020*

Climate Science case study: Cloud Feedback and Climate Sensitivity

BER scientists led the effort to quantify cloud feedbacks, constrain climate models, providing a major element in the international effort to pin down Equilibrium Climate Sensitivity (ECS)

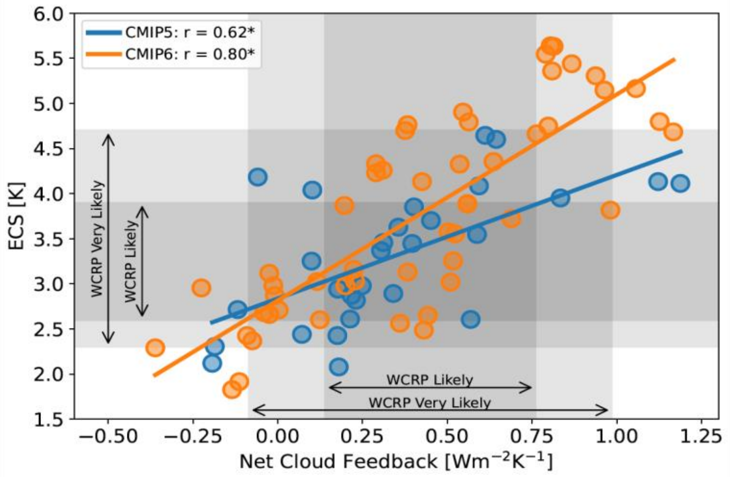


Figure shows ECS scattered against net cloud feedback for CMIP5 and CMIP6 models. Overlain shading indicates the very likely (90%) and likely (66%) total cloud feedback and ECS from a new estimate by BER scientists. Figure modified from Fig. S4 of Zelinka et al. (2020)

- Developed the innovative ***Cloud Radiative Kernel*** technique (Zelinka et al. 2012a,b) to quantify cloud feedbacks. Results featured prominently in IPCC AR5
- Discovered ***Emergent Constraints*** to constrain model predictions by decomposing the overall cloud feedback into tangible mechanisms testable by observations (Klein and Hall 2015).
- Among the leaders of the international effort that has ***reduced the uncertainty of ECS*** from the often-quoted 1.5–4.5˚C likely range to the narrower range of 2.6–3.9˚C.

Partnerships: Recommendations

- Develop new funding modalities to enhance international partnerships and cross-agency cooperation, such as by joint calls with NSF and other agencies
- Increase opportunities for engagement of BER program managers with their international counterparts
- Develop new international programs and consider establishing a formal office for international activities
- Increase fellowships, scholarships and international exchange opportunities
- Optimize resources and efficiencies by bridging across agencies and nations

Productivity: Findings

- BER user facilities, by virtue of their unique expertise, leadership positions, and ability to attract users, provide unique potential for integrating researchers from across BER
- The BRC model achieves strategically important BER mission goals and could be applied to other relevant research areas, such as environmental microbiomes: BRCs have excelled at building networks of researchers working toward a common goal with high productivity and impact because of their integrative focus
- There is a good balance between large center projects and exploratory single PI projects
- Team-based projects with researchers from academic institutions and DOE National Laboratories should be maintained
- Volatility and perceived volatility in funding levels and in FOA topics create challenges for recruitment and retention at all career stages, and for long-term productivity
- Untapped potential for science accomplishments to inform innovation and applied solutions, due to silos and mission-boundaries within DOE and across agencies.
- For collaborative climate science research across US agencies, it is worth thinking beyond the current USGCRP facilitation without allocated funding (see DestinE case study)

Bioenergy case study: Bioenergy Research Centers (BRCs)

The BRCs target fundamental science with the mission of enabling sustainable bioenergy and have been recognized as a flagship model for DOE science center management

- since late 2007, >4100 publications and >800 invention disclosures; collaborative publications (co-authors from separate institutions) are in higher impact journals
- remarkable innovation record of patents per research $, which is twice most federal programs
- successful in driving domestic multidisciplinary, multi-institutional collaborations on common science problems
- there is some gap in widespread deployment into industry; noting that the BER-BRC mission is enabling fundamental science

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 (BRCs*) 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 economic and environmental analyses for a sustainable biomass supply.	Develop "plants as factories" for biofuels and bioproducts.	Develop process and extraction technologies for plant oils and sugars.	Establish an automated biofoundry for fuels and bioproducts.
CBI	Optimize water and nutrient use in dedicated, high-yielding bioenergy crops.	Create genomic tools for accelerating the domestication of bioenergy crops.	Advance integrated and consolidated thermophilic bioprocessing.	Generate drop-in biofuels and bioproducts from biomass and lignin residues.
GLBRC	Conduct long-term studies of growing energy crops on nonagricultural land.	Design productive and high-value energy cropping systems.	Develop cost-effective biomass deconstruction and separation strategies.	Identify and engineer novel biomass conversion microbes.
JBEI	Study environmental resilience of engineered bioenergy crops.	Engineer plants for atom-economical conversion into biofuels and bioproducts.	Develop feedstock-agnostic biomass deconstruction processes using renewable ionic liquids.	Develop high-throughput biosystems design tools and hosts for scalable, atom-economical biofuels and bioproducts.

* CABBI: Center for Advanced Bioenergy and Bioproducts Innovation; CBI: Center for Bioenergy Innovation; GLBRC: Great Lakes Bioenergy Research Center; JBEI: Joint BioEnergy Institute.

Well-managed, stable, integrative, collaborative science can be highly successful in science impact and competitiveness.

Biodesign: People, Partnerships, & Productivity Findings

One of the projects awarded in 2017 under Funding Opportunity Announcement DE-FOA-0001650 (Biosystems Design)

Establishing a *Clostridia* foundry for biosystems design by integrating computational modeling, systems-level analyses, and cell-free engineering technologies

Northwestern University | LanzaTech | Oak Ridge National Laboratory

https://doi.org/10.1038/s41587-021-01195-w (2022)

◆ WSJ NEWS EXCLUSIVE | IPOS

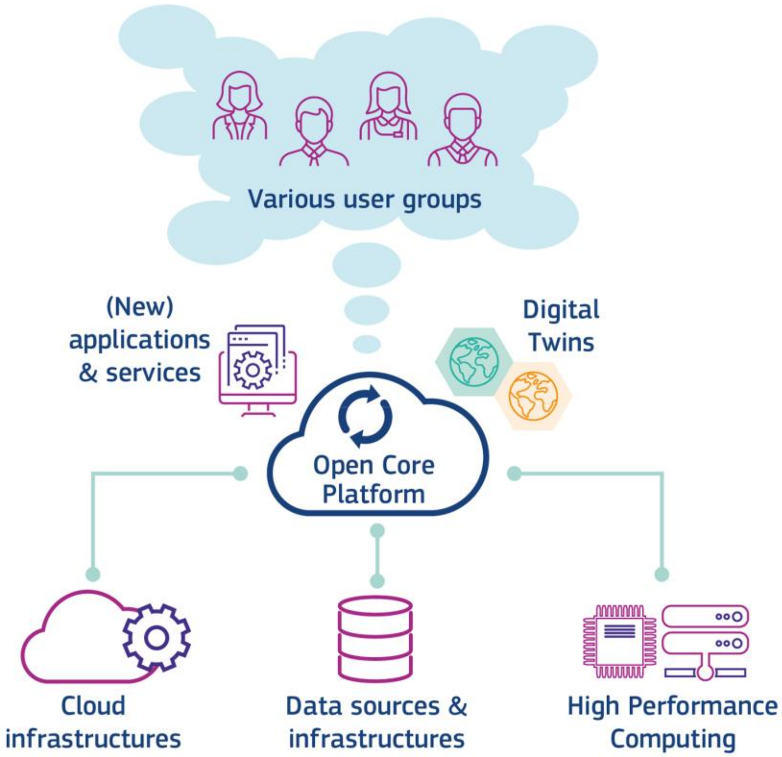
Carbon-Transformation Startup LanzaTech is Going Public in $2.2 Billion SPAC Deal

Company traps waste gas, uses bacteria to turn it into sustainable chemicals and products for customers including Unilever and Coty On March 8, 2022

Integration case study: Destination Earth

- Destination Earth (DestinE) is a major new integration initiative of the European Commission, with ≈$500M committed over the first 7–10 years
- Joining European scientific and industrial forces to develop a high precision digital model of the Earth to monitor and predict environmental change and human impacts interactively
- Goals to monitor and simulate Earth's land, marine, atmosphere, biosphere, and human interventions; anticipate socio-economic crises from environmental disasters for risk management; and aid agriculture's key functions in response to extreme weather

The new DestinE program is combining expertise under multi-agency leadership to dramatically improve delivery of integrated and interactive climate, ecosystem, and impacts science to public and private user groups.



https://digital-strategy.ec.europa.eu/en/policies/destination-earth

Productivity: Recommendations

- Reach beyond the silos, for cross-program, cross-division, and cross-agency action
- Cross-cutting organizations that support early and mid-career researchers (akin to the Max Plank groups in Europe, or Chinese institutes for environmental and climate science) may be an ideal way to encourage the most interdisciplinary topics, while building a productive, creative workforce
- Manage volatility, potential and realized, in funding levels and in FOA topics
- Inter- and intra-agency cooperation and co-funding could be used to foster interdisciplinary collaborations, maximize the use of large-scale resources such as field sites, and bridge Technology Readiness Levels (TRLs)
- Create a culture of communication and interaction across the TRL spectrum in DOE and among BER, businesses, and NGOs.
- Develop integrative science opportunities as a signature area for BER

Timeline

Date	Event	Actions
April 22nd	Spring BERAC	Presentation of key findings and recommendations
May 31st	WGs finalize chapter drafts	Report sent for editing
July 31st	Edited report ready	WG Co-leads and Co-Chairs review
August 30th	Final report ready	Co-Chairs submit report to BER
October	Fall BERAC	BERAC votes on approval of report

Reflections and Conclusions

- BER science and infrastructure is world-leading in its scale and scope
- For the coming decades, BER mission areas have a critical role at the nexus of global challenges of climate change, energy transitions and sustainable prosperity
- Investment across the mission areas needs to keep pace with the international research community, and better leverage integrative science across BER’s mission areas
- People are the most important resource – make cultural change to be the global attractor of top talent
- In a global research community, we are interdependent on others for our national success
- Scan the horizon often, avoid failures of inspiration and imagination

Failure is not an option