Discovery and Innovation for Biological and Climate Science at the Department of Energy

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(http://science.energy.gov/ber/)
1. Overview of the Department of Energy
2. Introduction to the Office of Biological and Environmental Research
3. Highlights and Opportunities for Discovery and Innovation
Biological and Environmental Research (BER)

Understanding complex biological, climatic, and environmental systems across vast spatial and temporal scales

The Scientific Challenges:

- Understand how genomic information is translated with confidence to redesign microbes, plants or ecosystems for improved carbon storage, sustainable biofuel production, and controlled biological transformation of nutrients and contaminants in the environment.

- Understand the roles of Earth’s biogeochemical systems (atmosphere, land, oceans, sea ice, subsurface) in determining climate so we can predict climate decades or centuries into the future, information needed to plan for future energy and resource needs.
BER research and user facilities are managed within and across two Divisions.

**Biological Systems Science**
- Todd Anderson, Director
  - Genomic Science
    - Bioenergy Research Centers
  - Mesoscale to Molecules
  - Facilities & Infrastructure
    - Joint Genome Institute
    - Structural Biology

**Climate & Environmental Sciences**
- Gary Geernaert, Director
  - Atmospheric System Research
  - Environmental System Science
  - Climate & Earth System Modeling
  - Facilities & Infrastructure
    - Environmental Molec. Sciences Lab
    - ARM Climate Research Facility
Biological and Environmental Research (BER)

**Foundational Science** - integrating observations and experimental capabilities with modeling for predictive understanding

Explore frontiers of genome-enabled biology
- Sustainable bioenergy resources
- Function & organization of plant and microbial systems
- Mechanisms and regulation of carbon storage in plant biomass and microbial communities
- Biosystems design
- Systems biology via data integration and analysis within a systems biology knowledgebase

Understand the effects of greenhouse gas emissions on Earth’s climate and biosphere
- World-leading capabilities in climate modeling
- Representation of clouds in climate models
- Direct/indirect effects of aerosols on climate
- Interactions of carbon cycle and climate
- Predictive understanding of terrestrial ecosystems, focus on sensitive systems, e.g., Arctic and tropics
Genomic Science

• Determine the genomic properties, molecular and regulatory mechanisms, and resulting functional potential of microbes, plants, and biological communities central to DOE missions.

• Develop the experimental capabilities and enabling technologies needed to achieve a genome-based, dynamic system-level understanding of organism and community functions.

• Develop the knowledgebase, computational infrastructure, and modeling capabilities to advance the understanding, prediction, and manipulation of complex biological systems.

Biosystems Design Tools for Plant & Microbial Systems

• Research to establish biological design rules will enable the predictive design of innovative natural and hybrid systems for clean energy production.
  • Synthetic biology methods
  • Genetic toolkits
  • Predictive integration of components and processes
  • Verify & validate computer-aided design toolkits
  • Testbeds to prototype performance and function
Bioenergy Research Centers—Innovation for Clean Energy

- Established in 2007; annual progress reviews
- Renewed for 5 years in September 2012.

**BioEnergy Science Center** (Oak Ridge National Lab)
- Strategic focus on overcoming biomass “recalcitrance”
- Goal of “Consolidated Bioprocessing” – one-microbe approach going from plants to fuel

**Great Lakes Bioenergy Research Center** (U. of Wisconsin, Michigan State U.)
- Goal of re-engineering plants to produce more starches and oils
- Using high throughput technologies to optimize chem/bio process for biomass deconstruction
- Major research thrust on sustainability of biofuels

**Joint BioEnergy Institute** (Lawrence Berkeley National Lab)
- Experimenting with new pretreatment process using room temperature ionic liquids
- Engineering *E.coli* and yeast to produce hydrocarbons, “green” gasoline, diesel, jet fuel

Technical workshop in 2005 articulated science challenges

- > 2100 publications
- DOE-funded Bioenergy Research Centers File
  500th Invention Disclosure - March 3, 2016
Engineered Lignin in Poplar Improves Wood Degradability

**Objective**
Engineer reduced recalcitrance into poplar cell walls

**Approach**
- Design modified lignin components with labile bond structures to improve degradability
- Express enzymes *in planta* to synthesize cell walls with modified lignin components
- Demonstrate improved sugar yields in modified plants

**Results**
- Engineered poplar strains grow indistinguishably from wild type
- Gene expression *in planta*, lignin component analysis and saccharification assays indicate demonstrate engineered reduced recalcitrance into poplar tissues

Direct conversion of plant biomass to ethanol by engineered *Caldicellulosiruptor bescii*

**Objective**
Combine cellulolytic activity and ethanol production in one bioprocessing step

**Approach**
- Use bioinformatics analysis and metabolic engineering techniques to modify cellulolytic *C. bescii* with ethanol-producing genes from *C. thermocellum*

**Result**
- Modified *C. bescii* able to degrade unpretreated cellulose and ferment the resulting sugars to ethanol
- Approach demonstrates a 2nd Generation CBP process for bioethanol production

Chung et al. (2014) “Direct conversion of plant biomass to ethanol by engineered *Caldicellulosiruptor bescii*”  
*PNAS* 111(24): 8931-8936 (Jun).
Evolved Hexose Transporter Enhances Xylose Uptake and Glucose/Xylose Co-utilization in Saccharomyces cerevisiae

**Objective**

Develop methods to broaden the use of sugars in the typical biomass mixture by *Saccharomyces cerevisiae*

**Approach**

- Import of five carbon sugars into the cell remains an important bottleneck
- *S. cerevisiae* strain BY4742 strain is engineered with a heterologous xylose utilization pathway
- Constructed strain is then subjected to a laboratory evolution regime with xylose as the sole carbon source.
- Several strains recovered with improved growth phenotypes.
- Genome resequencing identified a single amino acid change in the hexose transporter (*HXT7*) responsible for the evolved phenotype.

**Results/Impact**

- Constructed mutant (*HXT7*(F79S)) shows improved xylose uptake rates that allows the *S. cerevisiae* strain to show significant growth with xylose as the sole carbon source, as well as partial co-utilization of glucose and xylose in a mixed sugar cultivation.

Bioenergy Research Centers Open Competition

- Funding Opportunity Announcement DE-FOA-0001540 for team-based, multi-institutional, cross-disciplinary, integrated systems research centers.
  - Centers may focus on two or more focus areas
- Total requested budget of $90 million per year.
- Center annual budgets may range from $12.5M to $30M for up to 5 years.
- Open competition for domestic organizations as prime applicant; open to any organization as subawardee
  - Pre-applications due 6/17/2016
  - Applications due 9/30/2016
  - Selections in FY2017; centers begin in FY2018
A new strategy to prevent the proliferation of engineered organisms in the environment

Objective
Design a biocontainment mechanism that prevents the growth of engineered microbes outside the laboratory.

Approach
Essential genes in an E. coli strain with a “recoded” genome that lacks the UAG codon, were redesigned so that the proteins they code for require the incorporation of a specific non-standard amino acid (NSAA) in newly introduced UAG codons.

Results/Impact
- The redesigned proteins are functional and allow the cell to live and reproduce only if the NSAA is provided in the medium. The lack of that NSAA in natural environments prevents the modified strain from growing outside the laboratory.
- The investigators redesigned three essential genes within the same strain, reducing the number of reversion by mutation or by horizontal gene transfer to undetectable levels.
- The technology will advance toward the safe production of fuels and other chemicals in engineered microbial cells.

Mandell et. al. “Biocontainment of genetically modified organisms by synthetic protein design” Nature (online: January 21, 2015) doi:10.1038/nature14121
Enabling Technologies for Systems Biology

• Enable access for the biology community to structural biology beamlines and instrumentation at national user facilities (DOE BES light sources and neutron facilities; the Linac Coherent Light Source). Coordinated with BES and NIH.

• Develop capability to combine structural information on biomolecules with computation and/or bioinformatics to infer function and improve genome annotation or design new functions.

• Develop in situ, dynamic, and nondestructive approaches to multifunctional imaging, quantitative flux measurements, and multiscale integrative analysis of biological systems.

• Develop and support the DOE Systems Biology Knowledgebase (KBase), a Community Resource for Predictive Biology. This open-source and open-architecture computational environment will enable collaborative generation & sharing of systems biology data and workflows; perform large-scale analyses on a scalable computing infrastructure; model interactions between relevant organisms; propose new experiments to further refine the models.

http://www.kbase.us
The mission of the JGI is to provide genome sequencing, genome data acquisition, and genome analysis in support of the DOE mission needs in bioenergy, carbon cycling and biosequestration, and biogeochemical processes.

- Genome and metagenome expression and sequencing of microbes, plants, and other complex systems, such as microbial communities or the rhizosphere.

- Genome annotation, functional analysis and verification of genome-scale biological system models. Systems-level integration and validation of genomic data from multiple sequencing and functional analyses.

- Sequencing more than 120 Terabases of DNA per year.

- Data analysis and storage enhanced via a partnership with the National Energy Research Scientific Computing center (NERSC) at Lawrence Berkeley National Laboratory.
**Objective**
Sequence *Eucalyptus*, the most widely planted hardwood forest trees in the world

**Approach**
- Eucalypts are a globally important (>20M ha) resource for pulp, paper, biomaterials and bioenergy
- *E. grandis* was sequenced as representative example of this hardwood lineage.

**Result/Impacts**
- The *E. grandis* genome in combination with other hardwood genomes (*Populus, Citrus, Prunus, Vitis*) provides a comparative basis on which to understand the evolution of hardwoods
- *Eucalyptus* displays a wide diversity of specialized metabolites including terpenes among several other compounds useful for biofuels and biochemicals development

Climate and Energy

Greenhouse gases (GHG) are emitted during energy production... and climate change impacts energy production and the environment.

BER programs seek to:

• Understand the effects of GHG emissions on Earth’s climate and the biosphere through:
  – World-leading capabilities in climate modeling
  – Unique capabilities in cloud and aerosol observations and process research
  – Ecosystem level research on climate change impacts and the carbon cycle.

• Advance foundational science to support effective energy and environmental decision making
DOE’s Role in Climate Change Research

- DOE has been a leader in climate science since the 1950s, beginning with atmospheric transport and the relationship between CO$_2$ and climate change.

- Today’s research relies on unique SC user facilities, such as the Atmospheric Radiation Measurement (ARM) Climate Research Facility and the Leadership Computing Facilities, to develop predictive, systems-level understanding of climate change.

- DOE coordinates with other agencies through partnerships and through the U.S. Global Change Research Program.

DOE/SC research addresses:

- The three important uncertainties in the earth’s radiant energy balance—clouds, aerosols, and atmospheric greenhouse gases

- The relationship between climate change and critical ecosystems

- The climate-energy-water nexus through modeling, data analytics, and analysis

- Complexity of the climate and earth system, that demands extreme scale computing
BER is tackling the major knowledge gaps in climate models

- Representation of **clouds** in climate models
- Direct and indirect effects of **aerosols** on climate
- Interactions of the **carbon cycle** and climate
Climate system components
Climate Impacts of Large-Scale Biofuels Expansion

Objective: Investigate how land-use policies and economic factors influence where and how biofuel crops are planted, the ramifications for land-use change and greenhouse gas emissions, and how these influence climate.

Approach: This study uses the DOE-supported Integrated Global Systems Model (IGSM) to model the climate effects of two global biofuels programs—one that allows conversion of natural areas to meet the increased demand for land, and a second that encourages more intense use of existing managed land, and restricts deforestation.

Results:
• Increased biofuel crop cultivation has negligible effect on global temperature.
• Significant regional warming will occur, up to 1.5 °C in the Amazon and Central Africa.
• Warming driven by forest clearing for cropland, strongly limited by degree of deforestation.

Accelerated Climate Model for Energy (ACME)

As one of the three major US climate model research centers, ACME is a DOE multi-laboratory project designed to accelerate the assimilation of advanced software, numerical methods, and advanced high resolution physics, to study extreme phenomena in a warming climate.

Unique, world-leading capabilities

- Highest spatial resolution of all climate models in the world
  - Resolution at 15-25 km in fully coupled mode
  - Resolution below 10 km, using advanced adaptive-mesh for specific regions
- Will be the first climate model compatible with next generation computer architectures, as they become available.

Science to assimilate into ACME

- Carbon cycle, with dynamic ecology, biogeochemistry, and land-atmosphere fluxes
- Detailed studies of the cryosphere: permafrost; ice sheets
- Detailed validation of ecosystem component models, using data from DOE field projects in the Arctic and Tropics
- Uncertainty quantification for full system and its components
- Focus in FY 2017: Testing with Large-Eddy-Simulation, based on high resolution details obtained from the DOE Atmospheric Radiation Measurement Facility to better predict extremes

Begun in 2014, involves 7 National laboratories and the National Center for Atmospheric Research (NCAR).
Next-generation Ecosystem Experiments (NGEE)

NGEE—coordinated projects coupling terrestrial field experiments and process modeling to more rapidly improve the representation of terrestrial ecosystem processes in Earth system models thereby improving the quality of climate model projections.

- Target regions chosen are globally important, climatically sensitive, and understudied/underrepresented in predictive models.
- NGEE projects combine field and laboratory studies, observations, and multi-scale model simulation, coordinating with ARM mobile campaigns.
- **NGEE-Arctic** (FY2012-2022): Warming of permafrost soils will release vast amounts of CO₂ and/or CH₄ to the atmosphere—a strong positive feedback to warming.
- **NGEE-Tropics** (FY2014-2023): Rainfall stress on tropical ecosystems and release of biogenic aerosols impact cloud condensation nuclei.
Environmental Molecular Sciences Laboratory – A DOE User Facility

EMSL’s suite of over 75+ premier experimental capabilities enables molecular-scale experimental and theoretical research on aerosol chemistry, biological systems, geochemistry/biogeochemistry, and interfacial and surface science.

Biosystem Dynamics and Design – Understanding and optimizing the response of organisms and biological communities to their environment.

Atmospheric Aerosol Systems - Molecular-scale understanding of key chemical and physical properties of aerosols to improve the prediction of climate models.

Terrestrial and Subsurface Ecosystems - The dynamics of nutrients, metabolites, and contaminants at biogeochemical interfaces in heterogeneous environments across scales.

Energy Materials and Processes – Understanding the physical and chemical properties of interfaces to design new materials and systems for sustainable energy applications.
Tackling Major Climate Uncertainties

Atmospheric Radiation Measurement (ARM) Climate Research Facility

- Provides the world’s most comprehensive 24/7 observational capabilities for obtaining atmospheric data for climate change research.
- Data has transformed understanding of aerosol-cloud interactions. Built most advanced parameterizations of atmospheric radiative transfer. Advanced radars provide unprecedented data on cloud motions and structure.
- Facility operates highly instrumented ground stations worldwide studying cloud formation, aerosol processes and their influence on radiative transfer.
- In FY 2017, ARM will continue to support its long-term measurements at fixed sites, and the mobile facilities will be deployed to three climate-sensitive regions demanding targeted measurements. The first mobile facility will study cloud-aerosol interactions in the marine boundary layer; the second will be deployed to Antarctica; the third will continue the experiment in Oliktok, Alaska.

The challenge of studying radiative transfer on land-ice-atmosphere-water in the Arctic
DOE Scientific User Facility
ARM Climate Research Facility

Provides continuous field measurements and data products that improve cloud and aerosol science in climate models.
New Insights into Ice Formation in Clouds

Objective: Understand how ice crystals form from aerosol particles.

Approach and Results:

- Multi-institutional team obtained samples of particles that act as ice nuclei from central California (ARM/CARES campaign).
- Used EMSL micro-spectroscopy and chemical imaging methods to characterize the physical and chemical properties of individual particles.
- Results demonstrate that ice-nucleating particles are not distinct from other particles, and are not a “needle in a haystack” challenge.
- Factors such as particle abundance and surface area govern the ice nucleation rate and ice formation processes.

Significance and Impact:

- Disproves the traditional view that there are very few but exceptional particles in the atmosphere that can become ice nuclei.
- Cloud models must be further developed to account for properties of the entire particle population as well as individual ice-nucleating particles.

Participants: Stony Brook University, EMSL, Advanced Light Source at LBNL and University of the Pacific

BER strategic science directions are guided by input from the research community, scientific workshops, the National Science and Technology Council, the National Academy of Sciences and BERAC.
BER Funding Modalities

Grants to Academic/Private Institutions

- Response to specific targeted Funding Opportunity Announcements
- All proposals are merit reviewed, most by peer review panels
- Most awards are made to single investigators (or collaborative teams of investigators at multiple institutions)
- Collaborations between DOE labs and universities are encouraged
- Projects have a defined scope and project period

Scientific Focus Areas (SFAs) – Integrated Team Funding to DOE Labs

- In 2009, research programs map to broad BER research budget categories.
- SFAs must be coherent, cohesive, long-term programs that reflect coordination and collaboration among individual and teams of investigators across National Lab divisions and institutions.
- Strong management plans are essential
- Many SFAs include academic collaborators as subawards
- SFAs established by competitive merit review; progress is evaluated on annual basis and triennial peer reviews (often on-site)
How to get involved with DOE programs:

• Look for funding opportunity announcements (FOA’s) on our web site [http://science.energy.gov/ber/funding-opportunities/](http://science.energy.gov/ber/funding-opportunities/)

• Contact the DOE scientific program manager in your area of interest

• Look for opportunities to interact with the DOE National Laboratories

• Take advantage of a DOE Scientific User Facility

• Volunteer to serve as a reviewer for a DOE peer review panel

• Participate in a DOE research needs workshop
Biological and Environmental Research information resources

- Program information
  - http://science.energy.gov/ber/
  - http://genomicscience.energy.gov/program/aboutBER.shtml

- Workshops: provide community input and signal new research directions
  - http://www.sc.doe.gov/ober/BER_workshops.html

- Research abstracts
  - http://www.osti.gov/oberabstracts/search.adv.jsp

- Funding Opportunity Announcements
  - http://science.doe.gov/grants/announcements.asp
BER encourages its research community to seek scientific partnerships and new collaborations to accomplish mission goals.

Thank you!

http://science.energy.gov/ber/