

2016 Genomic Sciences Program Annual PI Meeting

Todd Anderson, Ph.D.

Director, Biological Systems Science Division,
Department of Energy, Office of Biological &
Environmental Research

March 7, 2016



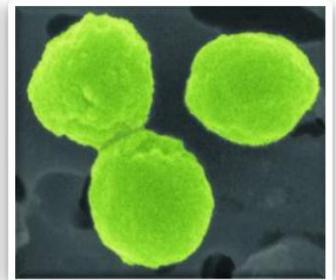
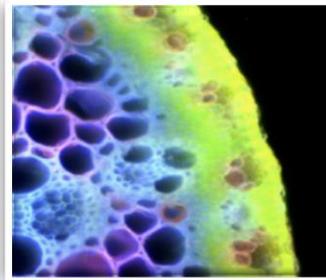
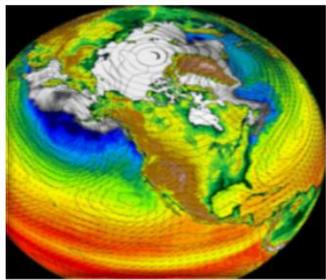
U.S. DEPARTMENT OF
ENERGY

Office
of Science

Office of Biological
and Environmental Research

DOE Biological & Environmental Research Missions

- Understand complex biological, climatic, and environmental systems across spatial and temporal scales.
- BER provides the foundational science to:
 - Support the development of biofuels as major, secure, and sustainable national energy resources
 - Understand the potential effects of greenhouse gas emissions on Earth's climate and biosphere and the implications of these emissions for our energy future
 - Predict the fate and transport of contaminants in the subsurface environment at DOE sites
 - Develop new tools to explore the interface of biological and physical sciences



Office of Biological & Environmental Research

Sharlene Weatherwax, Associate Director

Todd Anderson, Director

Biological Systems Science

- Genomic Science
- Bioimaging Technology
- Facilities & Infrastructure
 - Joint Genome Institute
 - Structural Biology

Gary Geernaert, Director

Climate & Environmental Sciences

- Atmospheric System Research
- Environmental System Science
- Climate & Earth System Modeling
- Facilities & Infrastructure
 - Environmental Molec. Sciences Lab
 - ARM Climate Research Facility

New Program Staff!

Dr. Dawn Adin – Microbiologist – Bioenergy



Dr. Ramana Madupu – Computational Biology



Dr. Amy Swain – Structural Biology/Bioimaging



BER FY 2016 Enacted

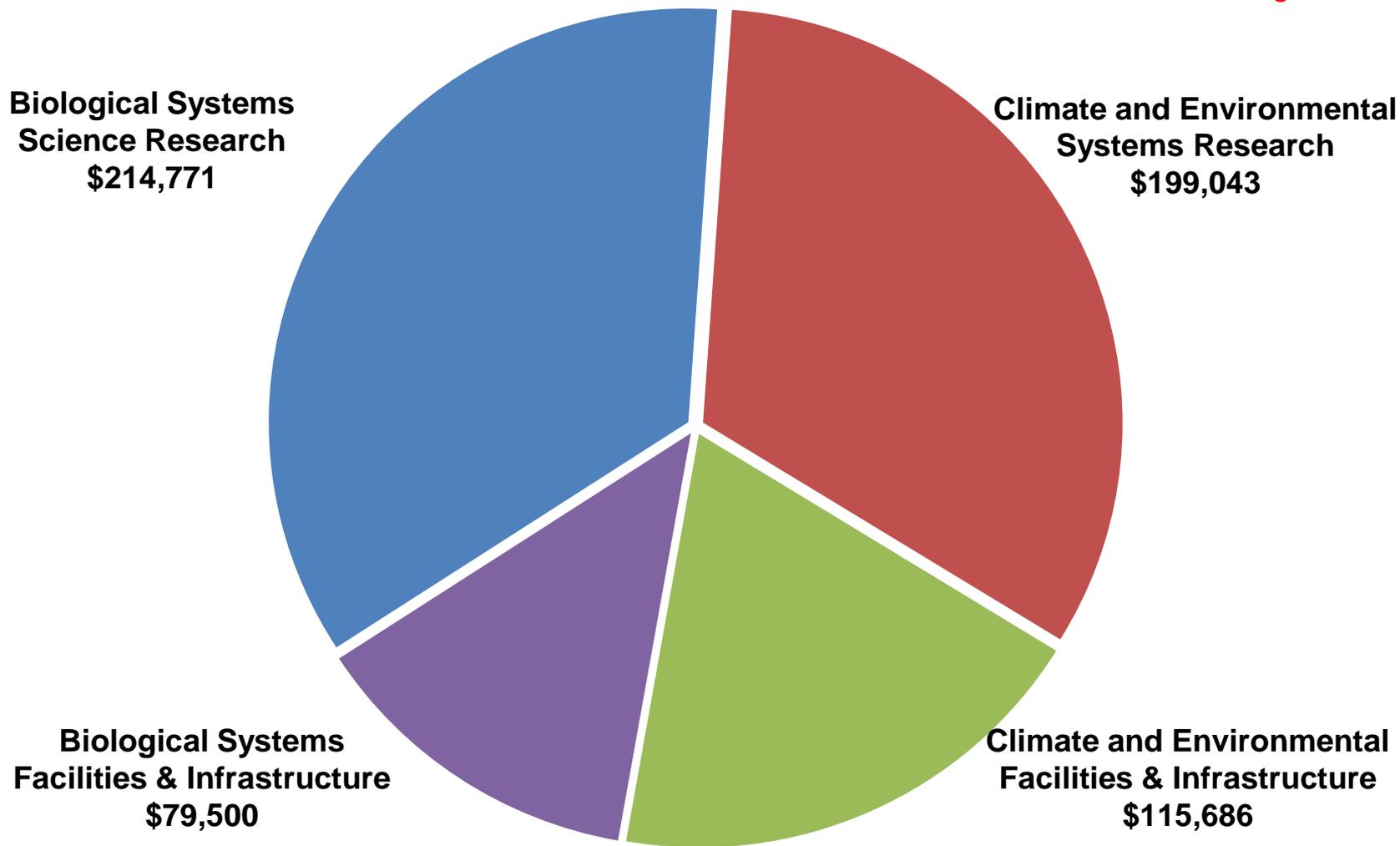
\$609,000 (\$612,400 President's Request)

(dollars in thousands)

At Request

+ \$32M

- Climate Modeling & Validation



BER FY 2017 President's Request

\$661,920

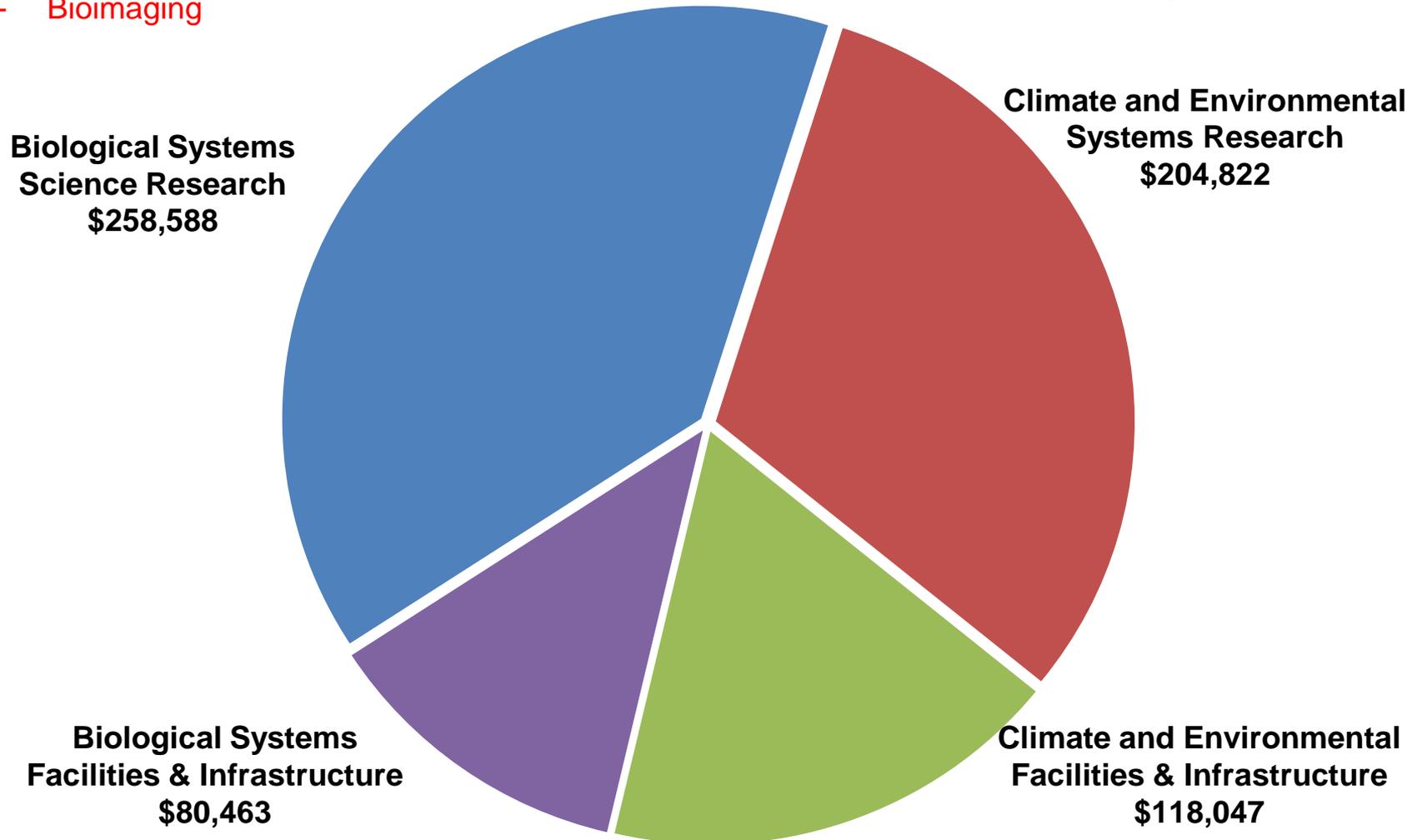
(dollars in thousands)

+ \$44M

- Mission Innovation
- Microbiome
- Bioimaging

+ \$8M

- Integrated Assessment



New FOAs for FY 2016

Plant Feedstock Genomics for Bioenergy: A Joint Research Funding Opportunity Announcement USDA, DOE (DE-FOA-0001444)

- *Continues research on plant responses to pathogens*
- *Includes a focus on oil seed crops*

BER Program Manager: Dr. Cathy Ronning

Systems Biology Enabled Research on the Roles of Microbial Communities in Carbon Cycle Processes (DE-FOA-0001458)

- *Research to understand the functioning of microbial communities in a wide range of environments and environmental conditions*
- *Research to inform larger scale ecosystem function*

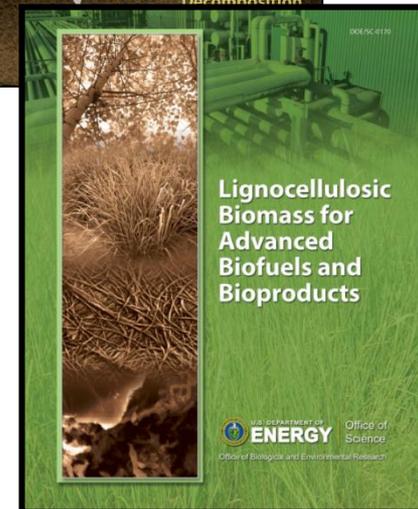
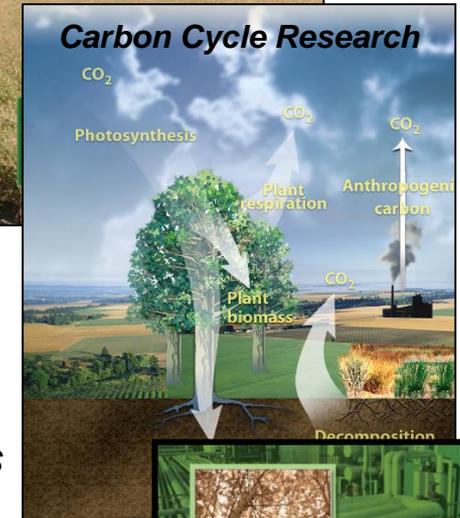
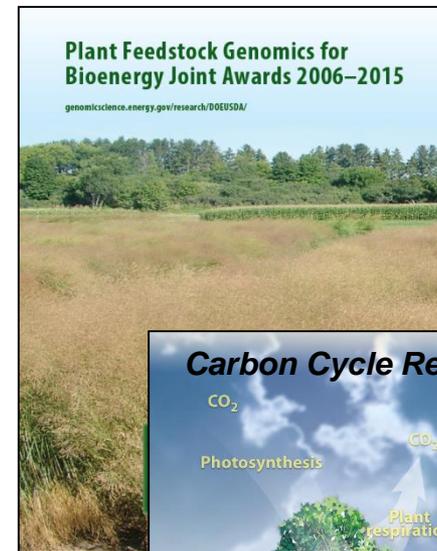
BER Program Managers : Dr. Joe Graber

Later this Fiscal Year

Bioenergy Research Centers FOA (open competition)

- *Informed by a recent BER workshop on bioenergy research*

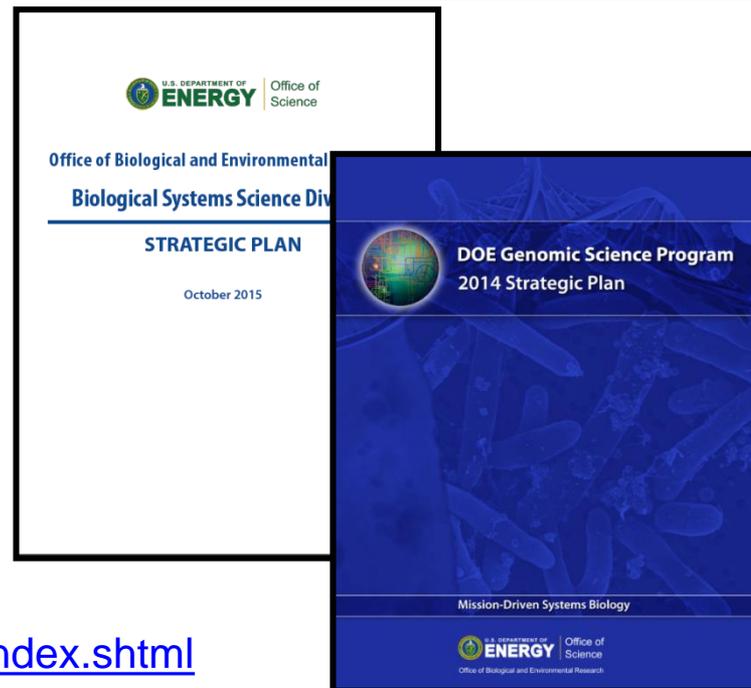
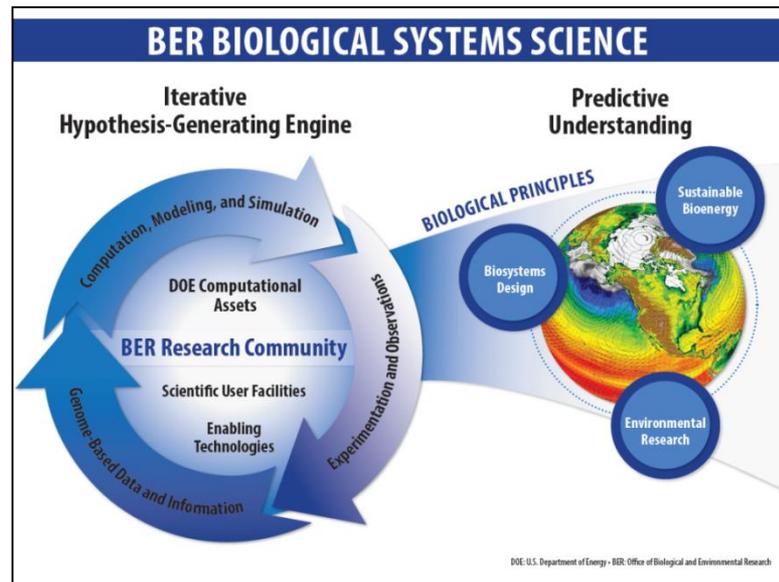
BER Program Managers : Dr. Kent Peters



Genomic Science Program

Main Program Components

- Bioenergy Research Centers (BRCs)
- Systems Biology for Bioenergy
- Plant feedstocks genomics*
- Biosystems design
- Carbon cycle/Environmental Microbiological research
- Computational biosciences
- Sustainability research for bioenergy



<http://genomicscience.energy.gov/strategicplan/index.shtml>

Bioenergy Research Centers (BRCs)



BioEnergy Science Center (Oak Ridge National Lab)

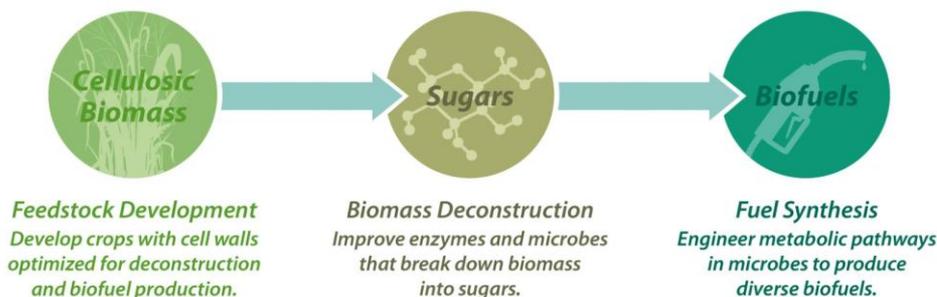
- Strategic focus on overcoming biomass “recalcitrance”
- Goal of “Consolidated Bioprocessing” – one-microbe or microbial community approach going from plants to fuel

Great Lakes Bioenergy Research Center (Univ. of Wisconsin, Michigan State Univ.)

- Goal of re-engineering plant cell walls for improved cellulose extraction
- 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 processes using room temperature ionic liquids
- Engineering *E.coli* and yeast to produce hydrocarbons, “green” gasoline, diesel, jet fuel



BER Program Manager: Dr. Kent Peters

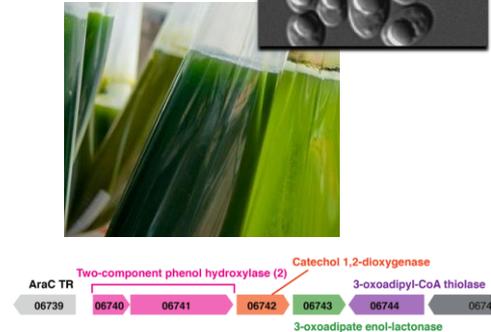
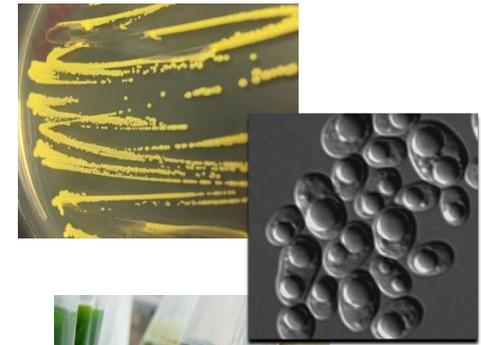
Systems Biology for Bioenergy

Fundamental, systems-level understanding of microbes and microbial communities relevant to advanced biofuels production.

- Research to advance the development of promising new model organisms relevant to biofuels production.
- Development of novel microbial functional capabilities and biosynthetic pathways relevant to the production of advanced biofuels and the development of strategies to overcome associated metabolic challenges resulting from pathway modification.
- Development of novel analytical technologies or high throughput screening approaches.

Broadens the portfolio in microbial research on advanced biofuels production

BER Program Manager: Dr. Dawn Adin



Genomic Science Program genomicscience.energy.gov

Systems Biology-Enabled Research for Microbial Production of Advanced Biofuels

Summary of Projects Awarded in 2014 Under Funding Opportunity Announcement DE-F00-0001660

The U.S. Department of Energy's (DOE) Genomic Science program, managed within the Office of Biological and Environmental Research (BER), supports fundamental research to identify the foundational principles that drive biological systems. These principles govern translation of the genetic code into organized networks of proteins, enzymes, regulatory elements, and metabolic pools underlying the functional processes of organisms. To address DOE's mission in sustainable bioenergy development, the Genomic Science program applies "omics"-driven tools of modern systems biology to challenges associated with microbial production of advanced biofuels.

Developing an increased understanding of how biological systems function and translating that knowledge to enhance the production capabilities of microbes and plants forms the basis of DOE's mission in sustainable bioenergy. To harness the microbial world's biosynthetic processing power for advanced biofuels production, an expanded set of platform organisms is needed with appropriate metabolic capabilities and stress tolerance characteristics. The DOE-BER Genomic Science program supports research aimed at improving fundamental understanding of principles that govern the functional properties of bioenergy-relevant organisms at the genomic scale. This knowledge will enable development of molecular genomics approaches and computational tools for the design, construction, and validation of improved biological components and systems. This highly interdisciplinary endeavor spans multiple fields in biology, systems biology, chemical and metabolic engineering, and computational biology.

Significant progress in the last decade has increased understanding of biological systems and the capabilities for manipulating them. These advances result largely from the tremendous technological leaps in developing molecular biology tools (e.g., genomics, metabolomics, and proteomics) used to analyze and modify the functional properties of biological systems. Despite these advances, many fundamental gaps remain in understanding microbial metabolism and physiology related to the production of sustainable, efficient, and economically competitive biofuels derived from lignocellulosic plant biomass or from photosynthetic capture of carbon dioxide (CO₂). The 2014 Funding Opportunity Announcement described herein specifically targets production of advanced biofuels, which in this context refers to biologically synthesized compounds with the potential to serve as energy-dense transportation fuels (e.g., diesel, gasoline, and aviation fuels) compatible with existing engines and fuel distribution infrastructure. Advanced biofuels production requires significant progress in the basic understanding of microbial metabolism and the conversion of photosynthetically derived carbon compounds (either via direct photosynthesis or acquired via breakdown of lignocellulosic plant biomass). Another goal is to determine how products can be efficiently shunted from central metabolism into complex products with associated rebalancing of organismal carbon allocations and redox potential.

BER solicited applications for systems biology-driven basic research in three areas of development focused on enabling advanced biofuels production:

- **Promising new model organisms relevant to bio-fuels production.** Proposed studies could include but are not limited to (1) advancing systems biology understanding and predictive modeling of specialist microbes or microbial consortia, (2) elucidating relevant regulatory and metabolic networks involved in product synthesis or environmental signal processing, (3) improving fundamental understanding of integrated function and compatibility of novel enzyme systems with direct applicability to lignocellulose breakdown or advanced biofuels production, and (4) developing genetic tools to facilitate study and manipulation of genetically tractable species.

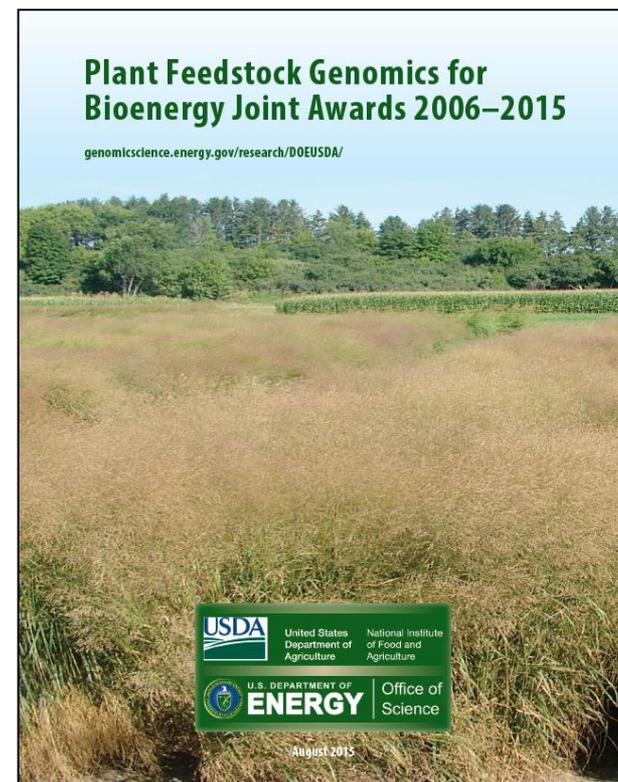
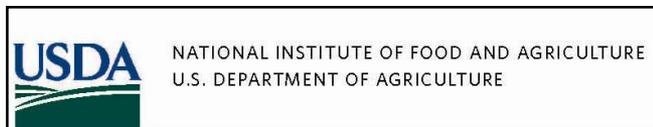
Office of Biological and Environmental Research Office of Energy Research

<http://genomicscience.energy.gov/biofuels/systemsbiology/microbialbiofuelsawardsflyer.pdf>

Plant Genomics Research for Bioenergy

Research to overcome the biological barriers to the low-cost, high-quality, scalable and sustainable production of bioenergy feedstocks using the tools of genetics and genomics

- Eleven-year collaborative effort with USDA on basic plant biology for bioenergy purposes
- Developing the scientific basis for new bioenergy crops
- Complementary with ongoing bioenergy research in BRCs and Biosystems Design
- New FOA includes plant responses to pathogens
- oil seed crop research



http://genomicscience.energy.gov/research/DOEUSDA/usda_doe_handout.pdf

BER Program Manager: Dr. Cathy Ronning

New Element! Sustainability Research for Bioenergy

Biosystems Design

Systems biology research applications focused on the design of new biological systems for bioenergy production.

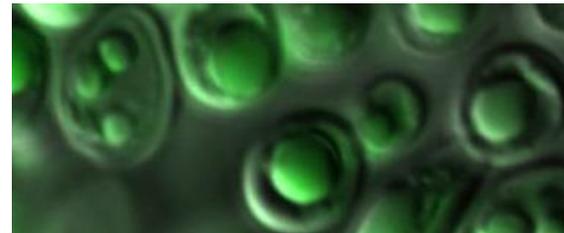
Microbial systems design for biofuels

- Integrated experimental and computational approaches aimed at designing flexible and tunable phototrophic or fermentative microbial systems for the production of advanced biofuels
- Novel genome-scale engineering to create new biological functions relevant to bioenergy production
- Development of innovative, exchangeable biological modules and/or organisms for engineering and, experimentally testing and validating re-designed microbial systems.

Plant systems design for bioenergy

- Systems-scale biology approaches to identify regulatory and metabolic modules that can be used to advance toward re-designing plants for increased photosynthesis capacity and biomass accumulation, as well as improved and sustainable nutrient and water utilization.
- New technologies for large-scale genome engineering of potential biomass feedstock plants as well as innovative techniques for the introduction of biological modules in plants to confer new or improved functions to bioenergy crops

BER Program Manager: Dr. Pablo Rabinowicz

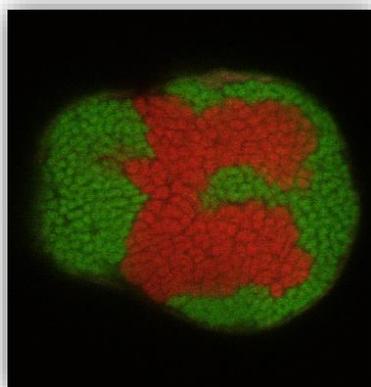


Environmental Microbiology

Genome enabled research linking structure and function of microbial communities with key environmental or ecosystem processes

- Systems biology of model microbes and consortia important in carbon cycle and environmental processes of relevance to DOE
- Extending systems biology approaches and understanding to integrated microbial communities and plant-microbe interactions
- Development of environmental “meta-omics” approaches to understand how shifts in environmental variables impact microbial community structure and functional processes
- High resolution, high throughput techniques for analysis of biological processes across multiple scales of spatial and temporal resolution
- Development of new techniques for in situ bioprocess analysis in terrestrial ecosystems

BER Program Manager: Dr. Joe Graber



Computational Bioscience

The DOE Systems Biology Knowledgebase A Community Resource for Predictive Biology



Open software and data platform for addressing the grand challenge of systems biology: **Predicting and designing biological function**

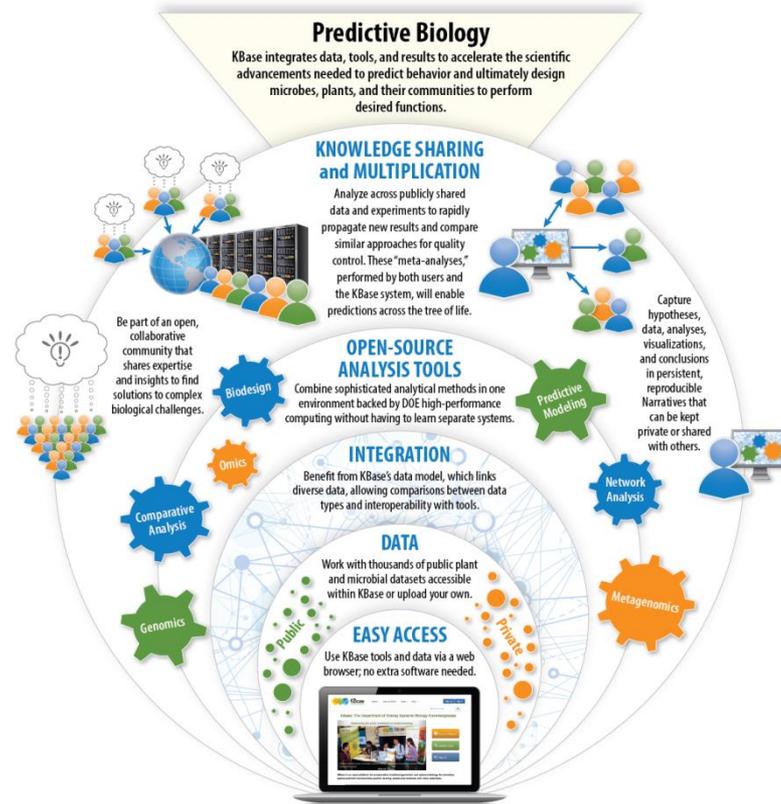


Unified system that integrates data and analytical tools for comparative functional genomics of **microbes, plants, and their communities**



Collaborative environment for **sharing methods and results** and placing those results in the context of knowledge in the field

New Feature! KBase TPT SDK v1 for Third Party Tool Integration



Demonstrations of the latest version at this Meeting!



DOE Systems Biology Knowledgebase

<http://www.kbase.us>

BER Program Manager: Dr. Ramana Madupu

Next Community Science Program (CSP) Call - OPEN

- Letters of Intent due: April 7, 2016
- Plant Functional Genomics and Microbiomes of DOE JGI Flagship Plants
- Function-driven Microbial Genomics
- Extreme Environments including Deep Subsurface
- Microbial Communities involved in Carbon and Nutrient (N,P,S) Cycling in Terrestrial environments

JGI-EMSL Collaborative Science Initiative - OPEN

- Letters of Intent due: April 4, 2016
- Biofuels and Bioproducts
- Plant-Microbe Interactions in the Context of Climate Change
- Biogeochemistry of Select Inorganic Elements of Interest to BER (metals,N,P)



Facilities Integrating Collaborations for User Science (FICUS)

- Link efforts among DOE User Facilities

<http://jgi.doe.gov/>

BER Program Manager: Dr. Dan Drell

Structural Biology Facility Access

X-ray Crystallography – atomic scale structure determination

- Structural Biology Center at the APS (Argonne) <http://www.sbc.anl.gov/>
- Structural Molecular Biology program at SSRL (SLAC) <http://smb.slac.stanford.edu/>

X-ray Scattering - rapid determination of overall shape of macromolecules and complexes:

- Structural Molecular Biology program at SSRL (SLAC) <http://www-ssrl.slac.stanford.edu/~saxs/>
- SIBYLS at the ALS (Berkeley) <http://www.bl1231.als.lbl.gov/>

X-ray Spectroscopy - oxidation state and speciation of elements in biomolecules:

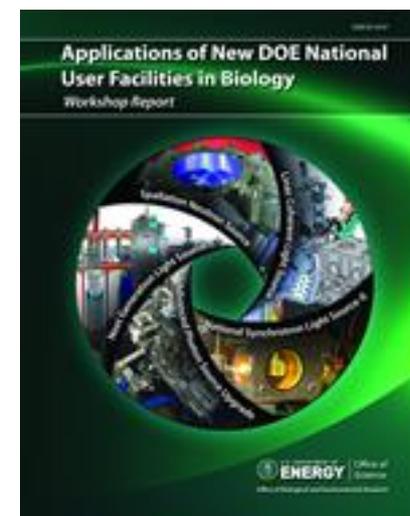
- Structural Molecular Biology program at SSRL (SLAC) <http://www-ssrl.slac.stanford.edu/~xas/>

Imaging at light sources - high resolution structures of living cells

- National Center for X-ray Tomography at the ALS <http://ncxt.lbl.gov/>
- Berkeley Synchrotron Infrared Structural Biology at the ALS <http://infrared.als.lbl.gov/content/structuralbiology>

Neutron Scattering - enables determination of shapes of proteins and complexes with high selective for specific features:

- Center for Structural Molecular Biology at HFIR (Oak Ridge) <http://www.csmb.ornl.gov/>



BER Program Managers: Dr. Roland Hirsch and Dr. Amy Swain

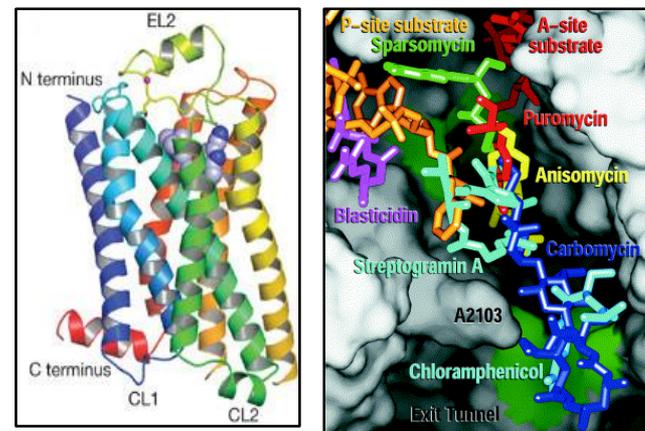
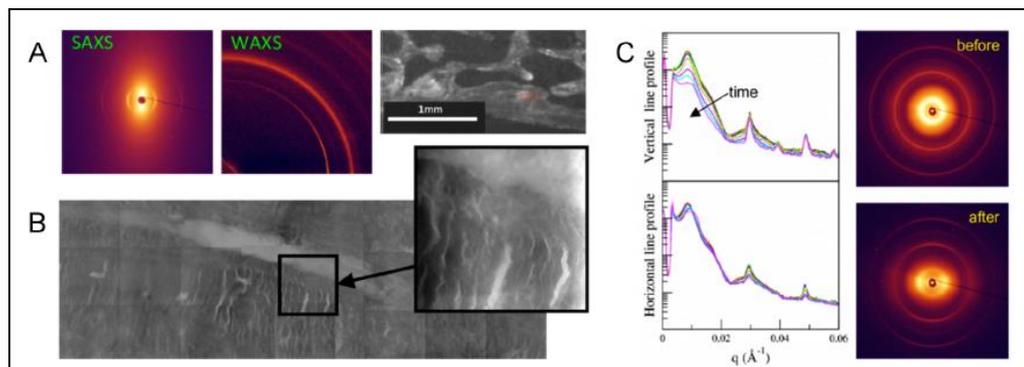
*NSLS-II ABBIX**

Life Science beamlines



**National Synchrotron Light Source II
(NSLS-II) at Brookhaven National Laboratory**

- ABBIX Project Goal: Build 3 state-of-the-art insertion device beamlines at NSLS-II for life science applications
 - Crystallography Beamlines:
 - AMX** -- Flexible Access and Highly Automated Macromolecular Crystallography
 - FMX** -- Frontier Macromolecular Crystallography
 - X-ray Scattering Beamlines:
 - LIX** -- High Brightness X-ray Scattering for Life Sciences
- Commissioning this spring
- Call for scientific community user proposals has been issued (<https://www.bnl.gov/ps/userguide/proposals.php>)



*(Advanced Beamlines for Biological Investigation with X-Rays)

Advancing discovery and mechanistic understanding of molecular-scale biological, chemical and physical processes and interfaces to enable predictive understanding of larger scale biological, environmental and energy challenges.

Providing access to multiple state-of-the-art instruments and high performance computing (HPC) capabilities to iterate between experimentation and modeling/simulation.

➤ **Proposal Opportunities:**

- Annual Science Theme LOI – due February 29, 2016 **Closed**
- Joint JGI-EMSL Call – due April 4, 2016 **Open**
- General and Scientific Partner – submitted anytime **Open**

➤ **Core Capabilities in:**

- Electron, Light and Specialized Microscopy
- Cell Isolation & Systems Analysis – bioreactors, single cell studies
- Mass Spectrometry – “omics”
- HPC – molecular dynamics/mechanics of biomolecules
- Liquid and Solid State NMR & EPR – Macromolecular assemblies/membrane proteins

Web Site and Call Info: <https://www.emsl.pnl.gov/emslweb/>

Virtual Tour: <https://www.emsl.pnl.gov/emslweb/facilities/virtual-tour>

BER Program Manager – Paul Bayer



Anaerobic gut fungi (Artistic rendering of the fungi by UCSB engineering graphic designer Peter Allen)



National Energy Research Scientific Computing Center

<http://www.nersc.gov/>

Energy Research Computing Allocations Process (ERCAP)

- 3B processor hours available at NERSC in FY15
- All Office of Science –funded PIs eligible to apply for compute time
 - 455M processor hours allocated to BER for FY16
 - **90M** processor hours for Biological Research
- New proposals accepted throughout the year for start-up time
- Production projects solicited in the Fall for larger compute requirements



Edison – Cray XC30



Cori – Cray XC (phase 1)

Apply for Your First NERSC Allocation

Initial Steps Needed to Apply for Your First NERSC Allocation

All work done at NERSC must be within the DOE Office of Science mission. See the Mission descriptions for each office at [Allocations Overview and Eligibility](#).

Prospective Principal Investigators without a NERSC login need to fill out two forms:

1. The online [ERCAP Access Request Form](#). If you wish to designate another person to fill out the request form you may designate a "PI Proxy" on this form.
2. Complete and submit the online [Computer User Assessment form](#).

Once we receive your agreement form and activate your account, you will receive an email with a link that will allow you to set your initial password. That link will expire if not used within 72 hours. If the link has expired, you will need to call NERSC Account Support at 1-800-496-3772, ext 2, or 510-486-6812 to obtain a temporary password. You can call at any time, 24 x 7, and somebody will be here to assist you.

Startup Allocations

Many new NERSC projects begin with a Startup allocation, particularly if they are new to HPC or are not yet ready to run production codes on thousands of CPU cores. Startup awards are limited to 50,000 MPP hours (Cray Hopper equivalent hours) and are good for up to 18 months.

A request for a Startup project can be made at any time during the year; decisions for Startup requests are made by NERSC within one to three weeks after applying. All questions on the application form must be answered (for the Other Info section only if the questions apply to your situation), but startup requests require only brief answers to the Code Description and Data questions.

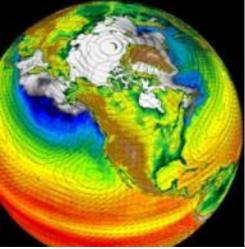
Startup awards are valid for up to 18 months (although they need to be renewed for a new allocation year) after which time the PI must obtain a "DOE production" award. This is accomplished by approval of the appropriate [DOE allocation manager](#) during the allocation year or by renewing the startup project as a production project for the next allocation year. Production projects are expected to have codes that use effectively one hardware to thousands of processors.

Submitting the Allocation Request Form

Requests to use NERSC resources are submitted on a web form. The process is known as ERCAP (Energy Research Computing Allocations Process). The ERCAP form is accessed through the NERSC Information Management (NIM) web interface.

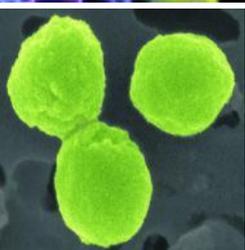
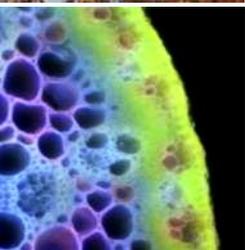
BER program manager:
Dr. Ramana Madupu

<http://www.nersc.gov/users/accounts/allocations/first-allocation/>



Systems science to meet DOE mission needs in bioenergy, climate and the environment.

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



Thank you!

<http://genomicscience.energy.gov>

