

# ***Biological Systems Science Division Update***

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U.S. DEPARTMENT OF  
**ENERGY**

Office  
of Science

Office of Biological  
and Environmental Research

# *Update Outline*

- Programmatic Actions
  - Updates
- Strategic Planning activities
  - Workshop
- Science highlights

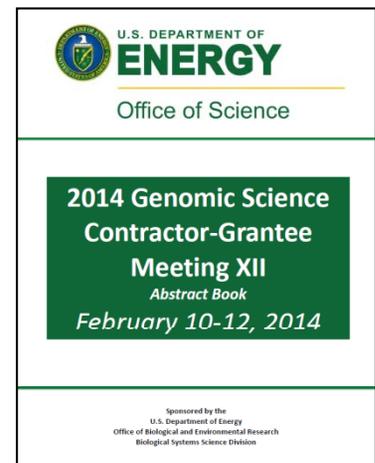
# Programmatic Activities

## Completed Reviews/Meetings

- Reviews of all three Bioenergy Research Centers
- Small Business Innovative Research (SBIR) review and award
- Early Career reviews – decisions pending
- Biofuels Science Focus Area (SFA) review
- Genomic Science Annual PI meeting (abstracts available)\*

## Upcoming Activities, Meetings and Reviews of DOE National Laboratory programs

- Lawrence Berkeley National Laboratory (Foundational Genomics SFA, April 1)
- Molecular Scale Science Challenges (May 27-29)
- Workshop on Bioenergy (June 23-25)
- Committee of Visitors review (July 9-11)



\* **Abstracts for PI meeting available at:**  
<http://genomicscience.energy.gov/pubs/2014summaries/index.shtml>

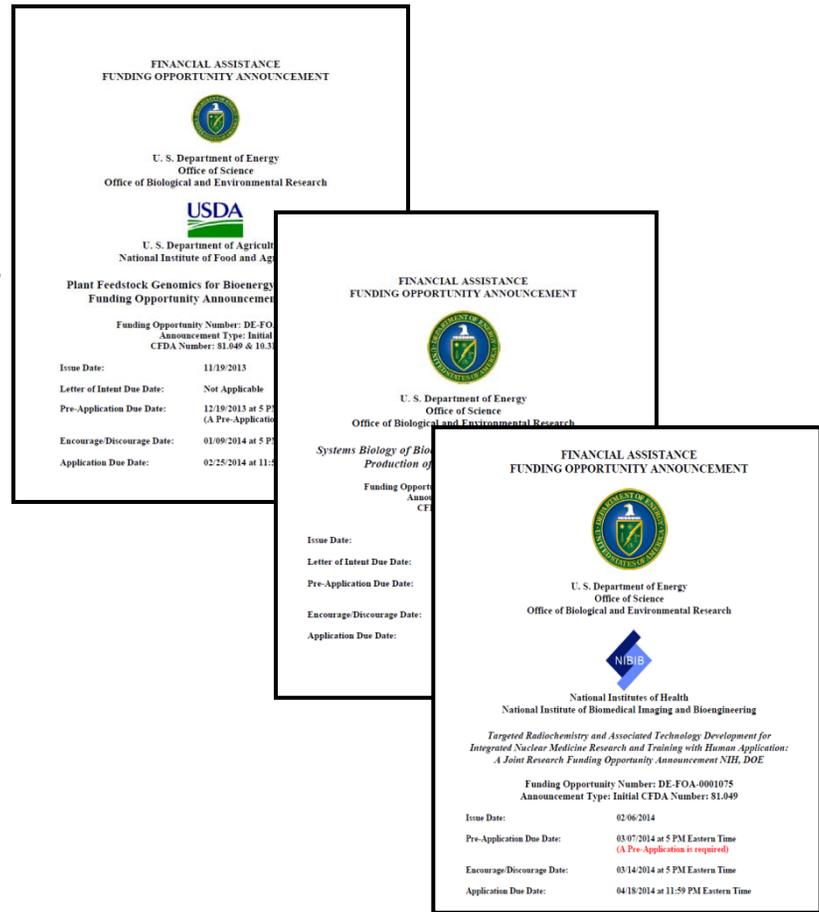
# New Notices

## ***Plant Feedstocks Genomics for Bioenergy: A Joint Research Funding Opportunity Announcement USDA, DOE (DE-FOA-0001034)***

- ***Full applications due February 25, 2014***
- Dr. Cathy Ronning**

## ***Systems Biology of Bioenergy-Relevant Microbes to Enable Production of Next Generation Biofuels (DE-FOA-0001060)***

- ***Full applications due March 14, 2014***
- Dr. Joe Graber**



## ***Targeted Radiochemistry and Associated Technology Development for Integrated Nuclear Medicine Research and Training with Human Application: A Joint Research Funding Opportunity Announcement NIH, DOE (DE-FOA-0001075)***

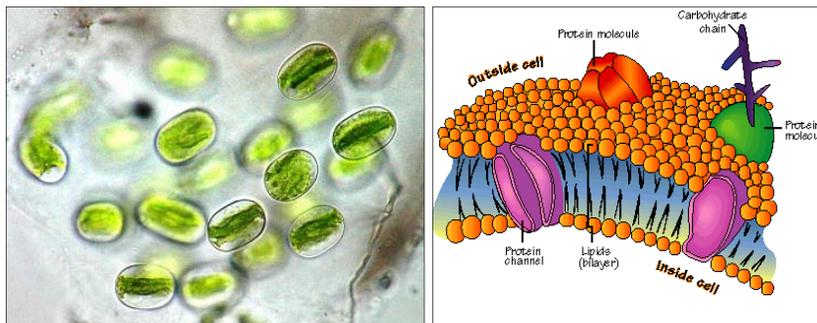
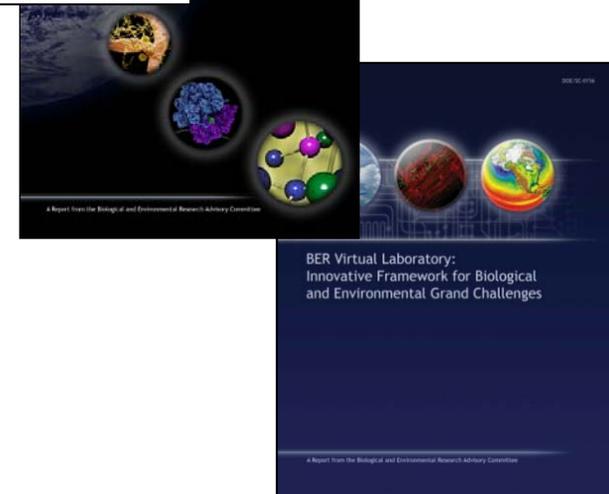
- ***Pre-apps due Mar 7, 2014***
  - ***Full applications due April 18, 2014***
- Dr. Prem Srivastava**

# Mesoscale to Molecules

- **Understanding translation of genomic information into the mechanisms that power living cells, communities of cells, and whole organisms.**
- **Imaging approaches to understand the genomic and physical rules governing formation and functions of subcellular mesoscale structures, the organelles and membranes in DOE relevant plants and microbes.**



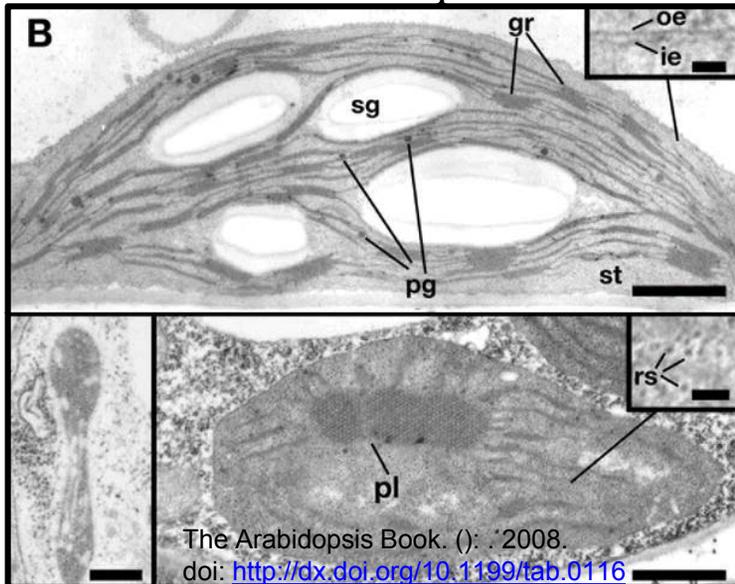
Grand Challenges for Biological and Environmental Research: A Long-Term Vision



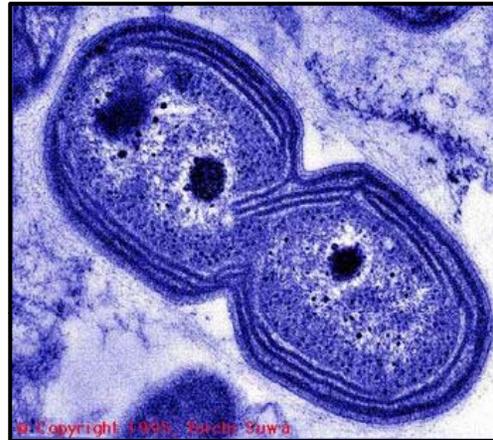
- **FY14 Pilot Projects at the DOE Labs**
- **Follow up in FY15 with an FOA**

# Mesoscale to Molecules

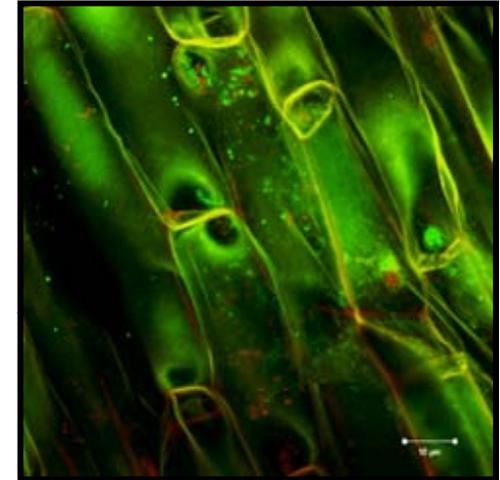
➤ *Material(s) Transport within and across Cellular Compartments*



➤ *Bacterial Cell Structure and Function*



➤ *Plant microbe interactions*



[http://www.esd.ornl.gov/PGG/weston\\_bio.htm](http://www.esd.ornl.gov/PGG/weston_bio.htm)

- .....
- Quorum sensing in microbial communities
  - Environmental signals impacting internal cell metabolism
  - Numerous other examples.....

***Multifunctional imaging/measuring techniques to translate static genomic information into the dynamic, systems biology context of whole cells, cellular communities and/or plant tissues.***

# Small Business (SBIR/STTR) Phase I Solicitation

## Six New Awards

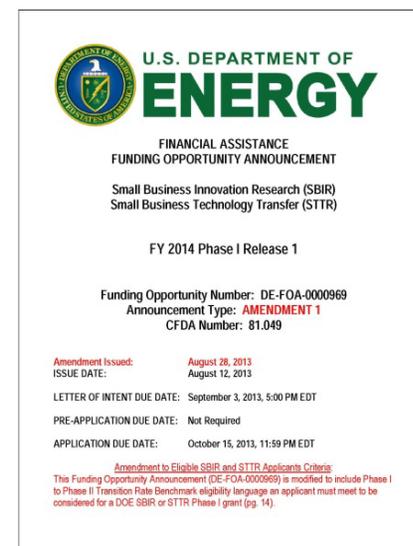
### Biofuels (Technology Transfer Opportunities)

- \* Improve lignin and cell wall characteristics in switchgrass, Afingen, Inc. (JBEI)
- Develop membrane dehydrators for ionic liquid recycling, Compact Membrane Systems, Inc. (JBEI)
- Develop microfluidic technology for engineering *E. coli* to produce fatty acid ethyl esters, HJ Science & Technology, Inc. (JBEI)
- Use *E. coli* to ferment sugars to C8 – C12 fatty acids, Technology Holding, LLC (GLBRC)

### Nitrous oxide sensors for biofuel sustainability

- Develop N<sub>2</sub>O sensor for eddy flux or soil chamber to include measurement of nitrogen isotopologue fluxes, Aerodyne Research, Inc.
  - \* Develop open path eddy covariance instrument for continuous and fast N<sub>2</sub>O emission measurements, Southwest Sciences, Inc.
- \* **“Fast-Track” – Combines Phase I and Phase II**

**Dr. John Houghton**



# *User Facility News*

## **Next Community Science Program:**

- Letters of Intent due 4/17/14
- Invited proposals due 5/27/14

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

## **JGI-EMSL Collaborative Science Initiative:**

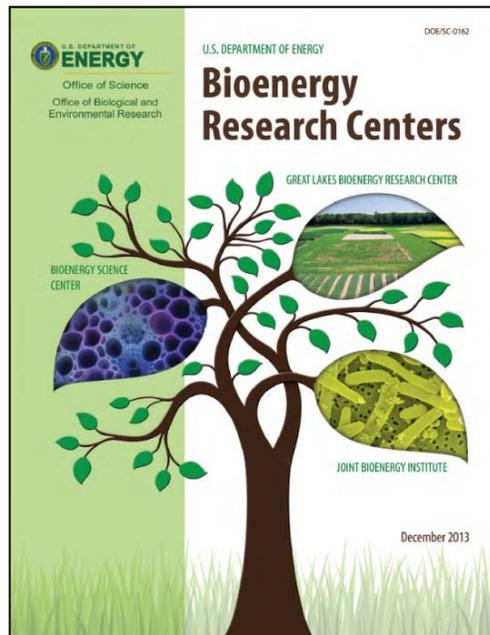
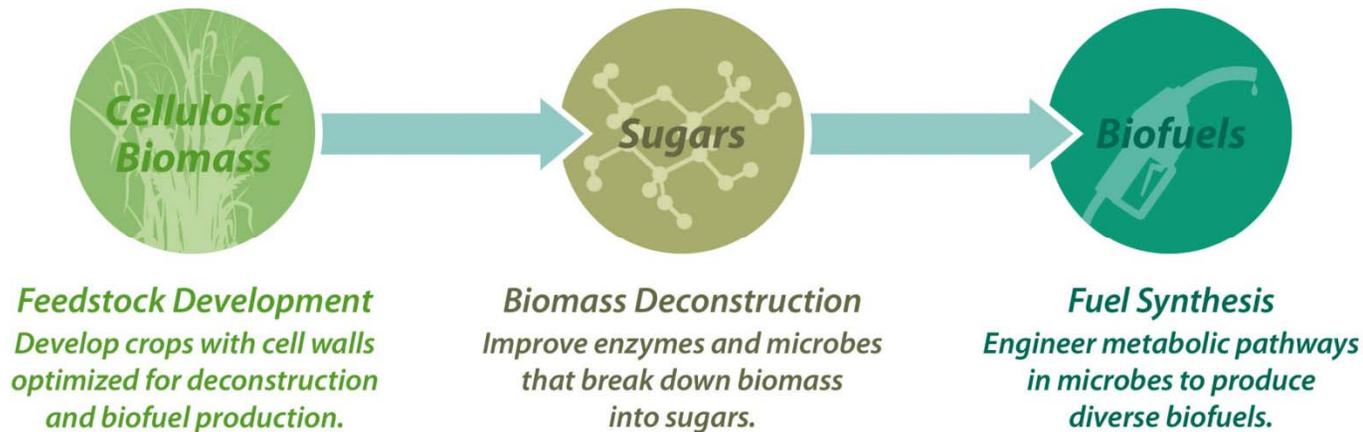
- Applications due April 7, 2014 at 11:00 p.m.

<http://www.emsl.pnl.gov/root/access/calls/jgi/2014/>



**Dr. Dan Drell**

# Bioenergy Research Center Brochure



- Updates scientific progress since the 2010 edition
- Revises each Center's scientific vision for research
- Provides a detailed list of significant published advances in the four major areas of emphasis at the Centers (including Enabling Technologies)

BER website link

<http://science.energy.gov/ber/news-and-resources/>

# Upcoming Workshops

## **Bioenergy Research**

*June 23-25, 2014 - Washington DC*

*Co-chairs: Dr. Kristala Jones-Prather (MIT)*

*Dr. Erich Grotewold (OSU)*

*Dr. Kent Peters*

## **Molecular Scale Science Challenges Workshop**

*(Joint with CESD)*

*May 27-29, 2014 – Washington DC Area*

*Co-chairs: Dr. Judy Wall (Univ. Missouri)*

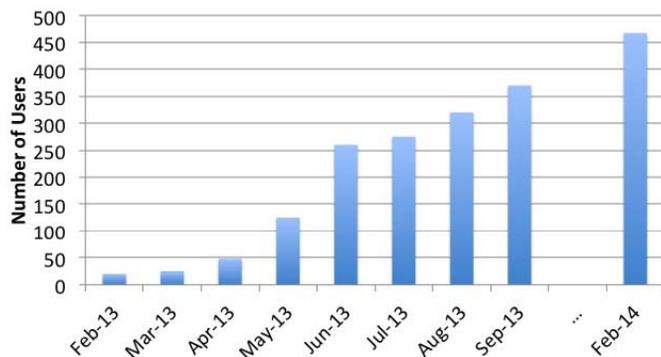
*Dr. James Liao (UCLA)*

*Dr. Roland Hirsch (BSSD)*

*Paul Bayer (CESD)*

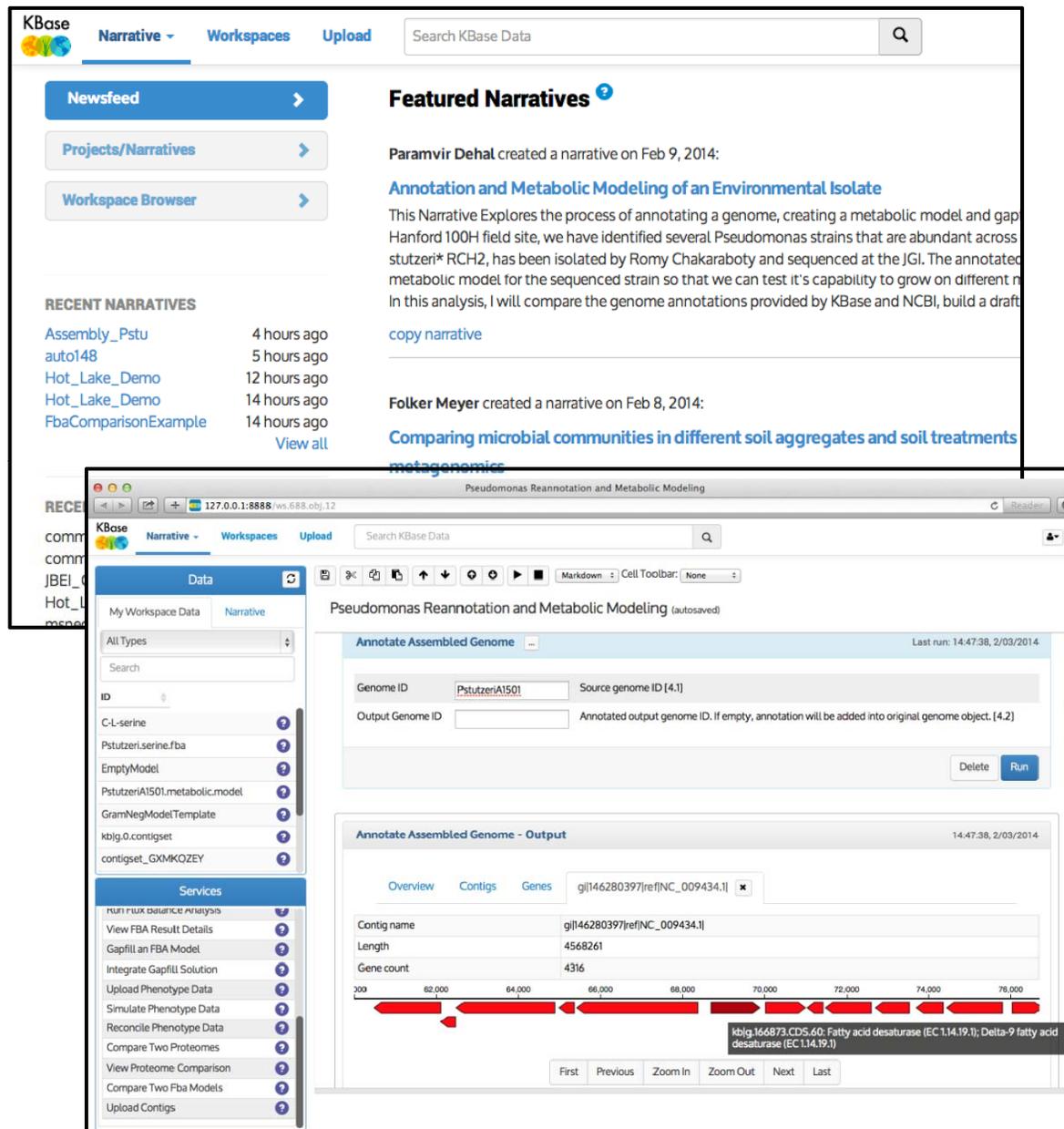
470 registered users  
(early adopter/tester group)

Growing User Base



*Graphical access to KBase tools and data. Researchers can create, modify, and share workflows, and reproduce the computational experiment of a Narrative with the push of a button.*

# Narrative Interface Rollout



The screenshot displays the KBase Narrative interface. At the top, there are navigation tabs for 'Narrative', 'Workspaces', and 'Upload', along with a search bar for 'Search KBase Data'. Below this is a 'Newsfeed' section with links to 'Projects/Narratives' and 'Workspace Browser'. The 'Featured Narratives' section highlights a narrative by Paramvir Dehal created on Feb 9, 2014, titled 'Annotation and Metabolic Modeling of an Environmental Isolate'. Below this, a 'RECENT NARRATIVES' list shows several entries with their creation times. The main content area shows a detailed view of a narrative titled 'Pseudomonas Reannotation and Metabolic Modeling'. This view includes a 'Data' sidebar with a list of workspace data items and services. The main workspace contains a form for 'Annotate Assembled Genome' with fields for 'Genome ID' (PstutzeriA1501) and 'Source genome ID' (4.1). Below the form is an 'Annotate Assembled Genome - Output' section showing a contig viewer for 'g|146280397|ref|NC\_009434.1|' with a gene count of 4316 and a genomic map showing gene locations.

# Chemical Factors that Control Lignin Polymerization

## Objective:

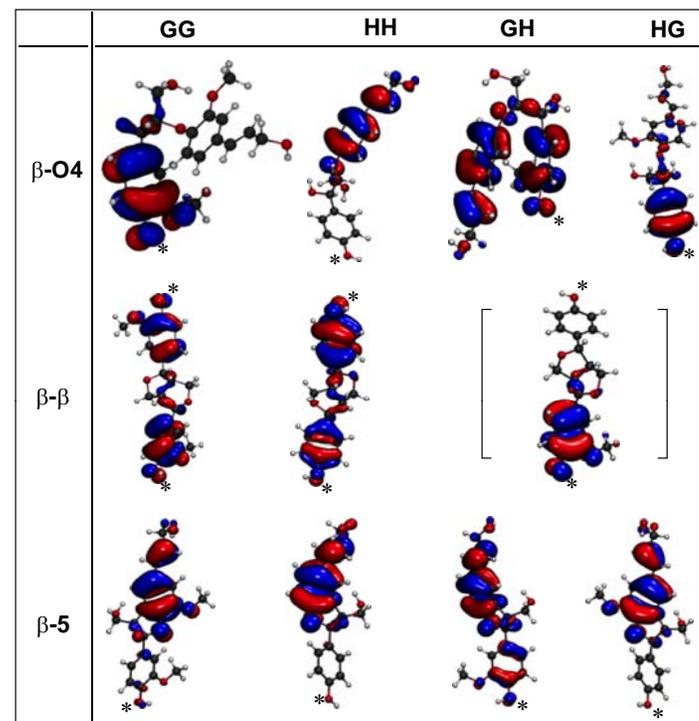
Lignin is a major contributor to biomass recalcitrance. Altering lignin composition in plant cell walls is an attractive approach to overcoming this recalcitrance. Increasing the content of para-hydroxyphenyl (H) subunits in lignin has been shown previously to increase sugar yields and reduce the size and molecular weight of lignin polymers. The objective of this study was to provide an explanation for why H subunits limit polymer growth.

## Approach:

Quantum chemical calculations were carried out to characterize the molecular orbitals and assess the reactivity of various mono-, di- and triligols that form natural lignins.

## Results/Impact:

- Results explain why H subunits in  $\beta$ - $\beta$  or  $\beta$ -5 linkages react poorly and tend to “cap” the lignin polymer.
- Provides a framework for understanding the propensity of different terminal subunits in lignin to undergo growth or termination.



HOMO electron density maps of homo- and heterodimers with  $\beta$ -O4,  $\beta$ - $\beta$  and  $\beta$ -5 interunit bonds (top to bottom). The magnitude of HOMO electron density on the phenolic oxygen correlates with the ability of the compound to undergo oxidation by HRP form a phenolic radical.  $\beta$ - $\beta$  GH and HG are identical by symmetry. Phenolic oxygens are indicated by an asterisk.

Sangha, A. K.; Davison, B. H.; Standaert, R. F.; Davis, M. F.; Smith, J. C.; Parks, J. M. “Chemical Factors that Control Lignin Polymerization,” *J. Phys. Chem. B*, 2014, in press.



## *High sugar production from plants using biomass derived solvent*

### **Objective:**

To avoid costly enzymatic or ionic liquid pretreatment of biomass by utilizing an organic solvent easily produced from biomass sugars to deconstruct biomass

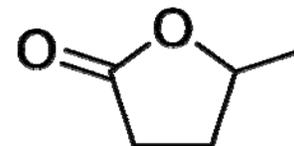
### **Approach:**

- Deconstruct biomass in a flow-through reactor with a residence time of 0.5-2 hrs at 127-200 °C
- Use liquid CO<sub>2</sub> or NaCl to obtain separate aqueous sugar, recycled GVL, and lignin streams

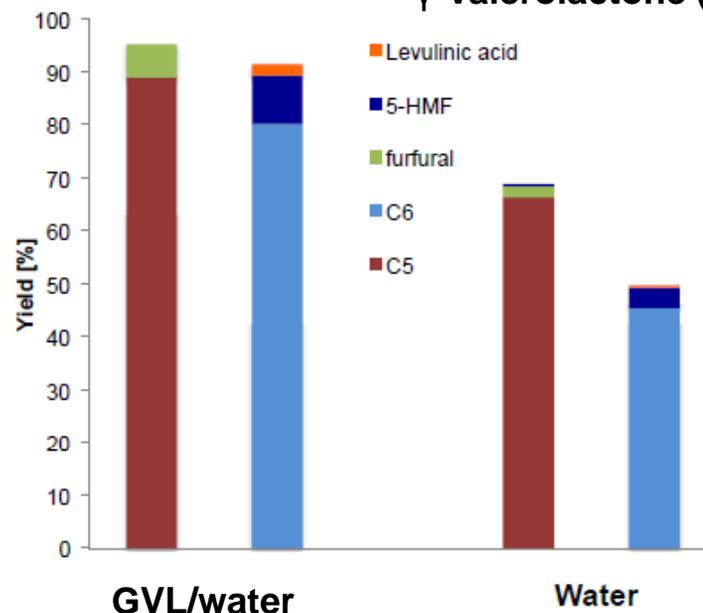
### **Result/Impacts:**

- High sugar recoveries (>90%) and low GVL contamination (<2%) in aqueous stream
- Aqueous stream can be used by microbes to produce ethanol at (>90%) yield
- Feedstock agnostic; works equally well with corn stover, maple, loblolly pine

Dumesic, J.A. et. al. 2014. *Nonenzymatic Sugar Production from Biomass Using Biomass-Derived  $\gamma$ -Valerolactone* **Science**, 343 (6168), 277-280.



$\gamma$ -Valerolactone (GVL)



# Engineering dynamic pathway regulation using stress-response promoters

## Objective:

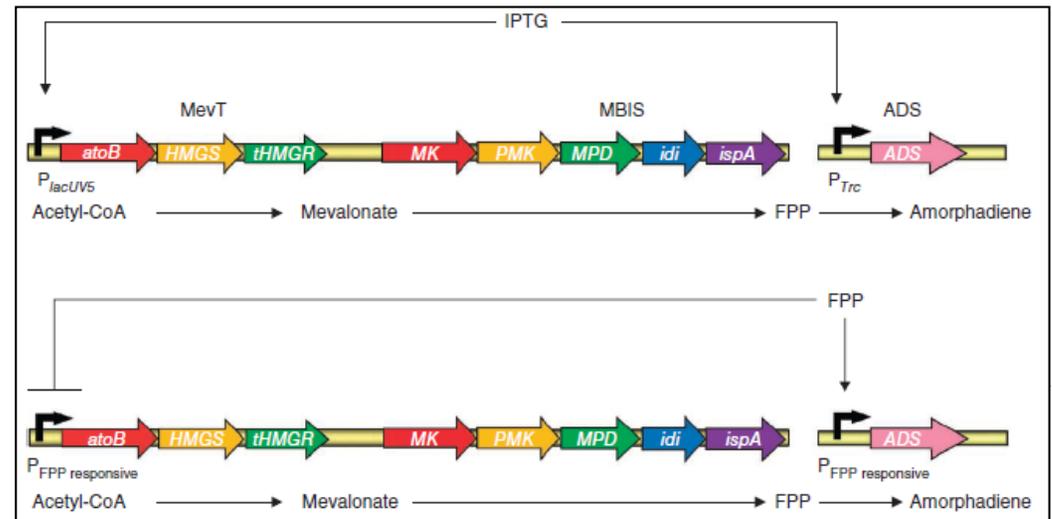
Genetically engineer pathways to be dynamically responsive to FPP concentrations

## Approach:

- Farnesyl pyrophosphate (FPP) is an intermediate in isoprenoid biosynthesis but is toxic to cells.
- Identify genes induced in response to FPP and use these gene promoters to drive biosynthetic pathway.

## Results/Impacts:

- Yields comparable to lac promoter controlled pathway
- Pathway is dynamically expressed in response to intermediate accumulation
- Demonstrated a technique for constructing dynamic pathway regulation independent of specific metabolite sensor
- Avoid use of expensive artificial gene inducers



Dahl, R., Zhang, F., Alonso-Gutierrez, J., Baidoo, E. E., Redding-Johanson, A. M., Batth, T. S., Mukhopadhyay, A., Petzold, C. J., Lee, T. S., Adams, P. D. and Keasling, J. D. (2013). "Engineering dynamic pathway regulation using stress-response promoters." **Nature Biotechnology** 31: 1039

## ***Discovery of a Novel Methanogen in Thawing Permafrost***

### **Objective:**

Characterize microbial community structure and functional processes at a permafrost-to-wetland transitional ecosystem in northern Sweden.

### **Approach:**

Deep metagenomic sequencing, metaproteomics, and methane flux measurements were used to characterize the microbial community and correlate members with *in situ* carbon cycle processes.

### **Results/Impact:**

- Assembly of nearly complete genome of Candidatus *Methanoflorens stordalenmirensis*, the dominant methanogen in thawing bog sites, from metagenomic libraries
- Coupled CH<sub>4</sub> flux measurement quantitative metaproteomic detection of *M. stordalenmirensis* methanogenesis proteins suggest that this organism dominates CH<sub>4</sub> production at bog sites.
- Methanogens closely related to *M. stordalenmirensis* are prevalent in metagenomic libraries for other thawing permafrost sites, suggesting global distribution in these ecosystems.



Mondav et al. 2014 **Nature Communications** DOI: 10.1038/ncomms4212

## **Parallel analysis of RNA ends (PARE) enhances global investigation of microRNAs and target RNAs of *Brachypodium distachyon***

### **Objective:**

Gain new insights into gene regulation via identification of microRNAs and microRNA cleavage targets in *B. distachyon*

### **Approach:**

- Isolate and sequence small RNAs from *B. distachyon* root, seedling, leaf, stem and stem tissue samples under a variety of drought, salt, cold, heat submergence conditions (17 sequence libraries in total)
- Screen and identify candidate microRNAs from sequencing data using a combination of computational (PARE) and experimental approaches
- Compare expression of identified microRNAs under the different tested conditions to gain insight on regulatory processes



### **Results/Impact:**

- Generation of an expanded microRNA and microRNA target dataset for *B. distachyon* from several samples and numerous environmental conditions
- Identified 116 microRNAs from 161 target sequences.
- Facilitate more detailed studies of gene regulation/validation in *B. distachyon*

Jeong D, et. al. (2013) *Parallel analysis of RNA ends enhances global investigation of microRNAs and target RNAs of Brachypodium distachyon* **Genome Biology** 2013, 14:R145 doi:10.1186/gb-2013-14-12-r145

# *Understanding the Thermal Pretreatment of Biomass*

## **Objective:**

To visualize the changes in the fine structure of biomass as it undergoes pretreatment in order to enable development of more efficient processing

## **Approach:**

Use a group of experimental tools to probe structure of the biomass during pretreatment and then carry out high performance computer simulations to develop a high-resolution picture of the biomass components. Wide angle X-ray fiber diffraction, Neutron fiber diffraction and time-resolved small-angle neutron scattering were used to study the biomass.

## **Results/Impact:**

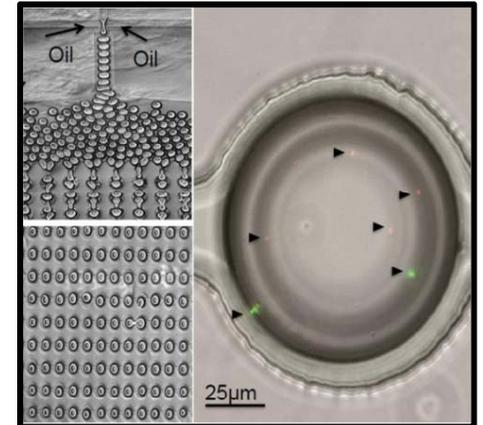
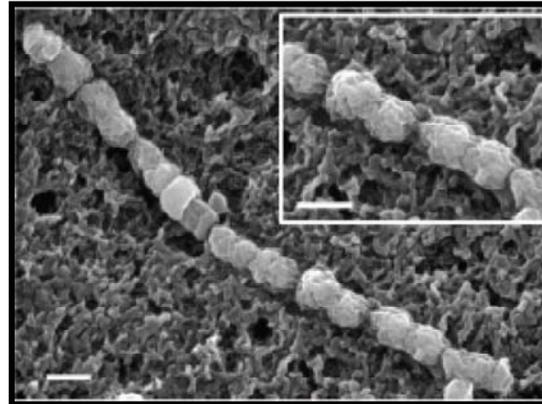
The research demonstrated these major changes in the biomass structure: cellulose dehydration, lignin-hemicellulose phase separation, and increased porosity of the cell wall matrix. The new understanding will enable improvements in biomass conversion processes.



Cover of the January 2014 issue of *Green Chemistry*, showing a simulation of the morphology of biomass during steam explosion pretreatment

Langan, P. et al. (2014) "Common processes drive the thermochemical pretreatment of lignocellulosic biomass", *Green Chem.*, 16, 63-68

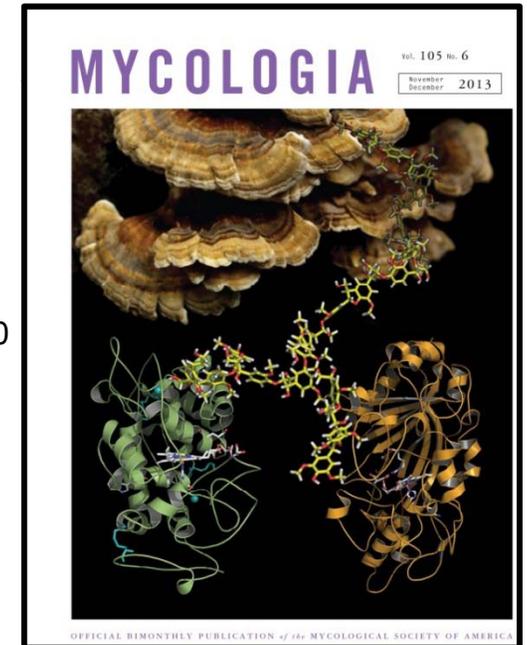
**Selected JGI Publications**



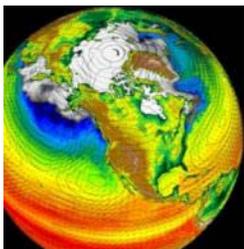
- Boscaro, V., et al. (2013) Polynucleobacter necessarius, a model for genome reduction in both free-living and symbiotic bacteria **PNAS** 110(46) 18590-5
- Jay, Z.J., et al. (2013) Predominant acidilobus-like populations form geothermal environments in Yellowstone National Park exhibit similar metabolic potential in different hypoxic microbial communities, **Appl. Environ. Microbiol.** doi 10.1128/AEM.02860 Epub 2013/10/29
- Lindemann, S.R., et al. (2013) The epsomitic phototrophic microbial mat of Hot Lake, Washington: community structure and responses to seasonal cycling, **Front. Microbiol.** 4323 doi:10.3389/fmicb.2013.00323
- Rice, D. et. al. (2013) Horizontal transfer of entire genomes via mitochondrial fusion in the angiosperm Amborella, **Science** 342:6165
- Tisserant, E. et al. (2013) Genome of an arbuscular mycorrhizal fungus provides insight into the oldest plant symbiosis, **PNAS** published ahead of print Nov 25, doi:10.1073/pnas.1313452110
- Hellstein U. et al., (2013) Fine scale variation in meiotic recombination in Mimulus inferred from population shotgun sequencing, **PNAS** Nov 26, 110(48):19478-82
- Haiwei, L. et. al. (2014) Single-cell genomics shedding light on marine Thaumarchaeota diversification **The Isme J.** 8:732-736
- Mukherjee, S. et al. (2014) Population level analysis of evolved mutations underlying improvements in plant hemicellulose and cellulose fermentation by *Clostridium phytofermentans*, **Plos One** 9(1)e86731 doi 10.1093.
- Wilson, M.C. et al. (2014) An environmental bacterial taxon with a large distinct metabolic repertoire. **Nature** Feb 6; 506(7486):58-62 doi:10.1038/nature2959 Epub 2014 Jan 29.

**37 publications since the last BERAC meeting**

JGI Publication Highlights: <http://www.jgi.doe.gov/News/pubs.html>

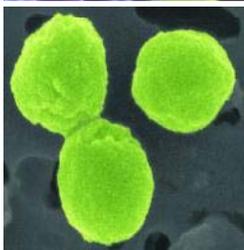
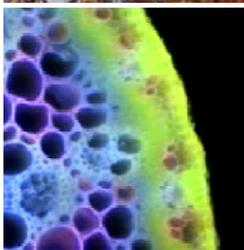


Cover of November/December issue of Mycologia, with JGI fungal phylogeny review



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

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



**Thank you!**

<http://genomicscience.energy.gov>



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