BioEnergy Science Center:
a DOE Bioenergy Research Center

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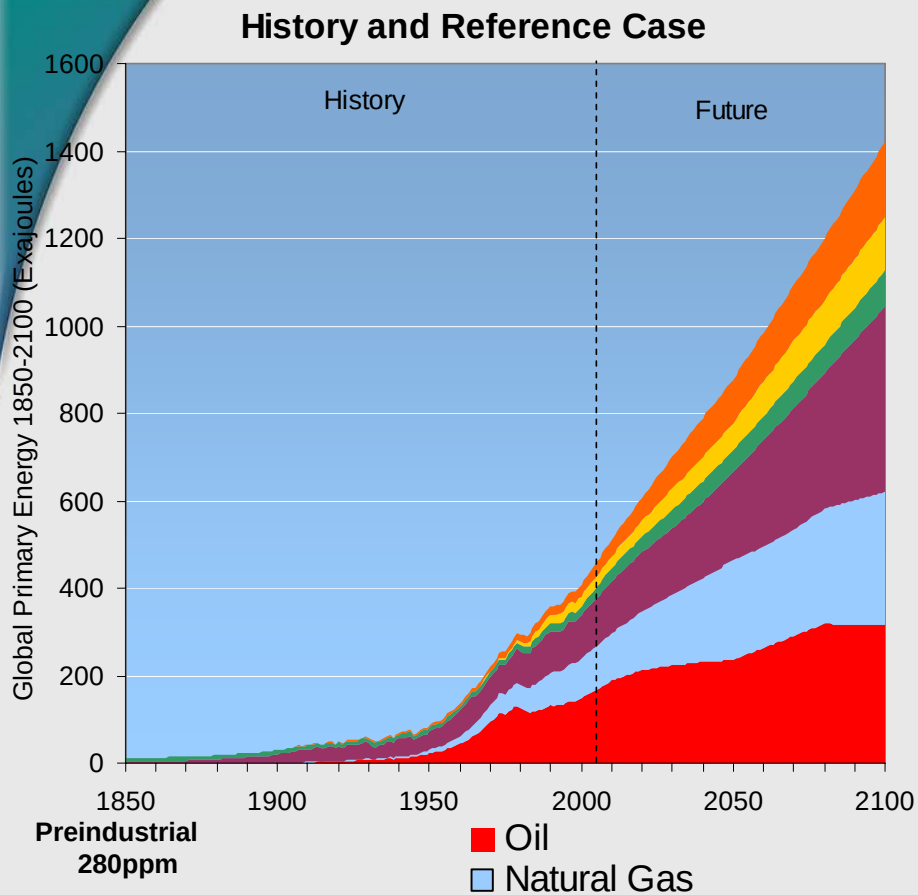
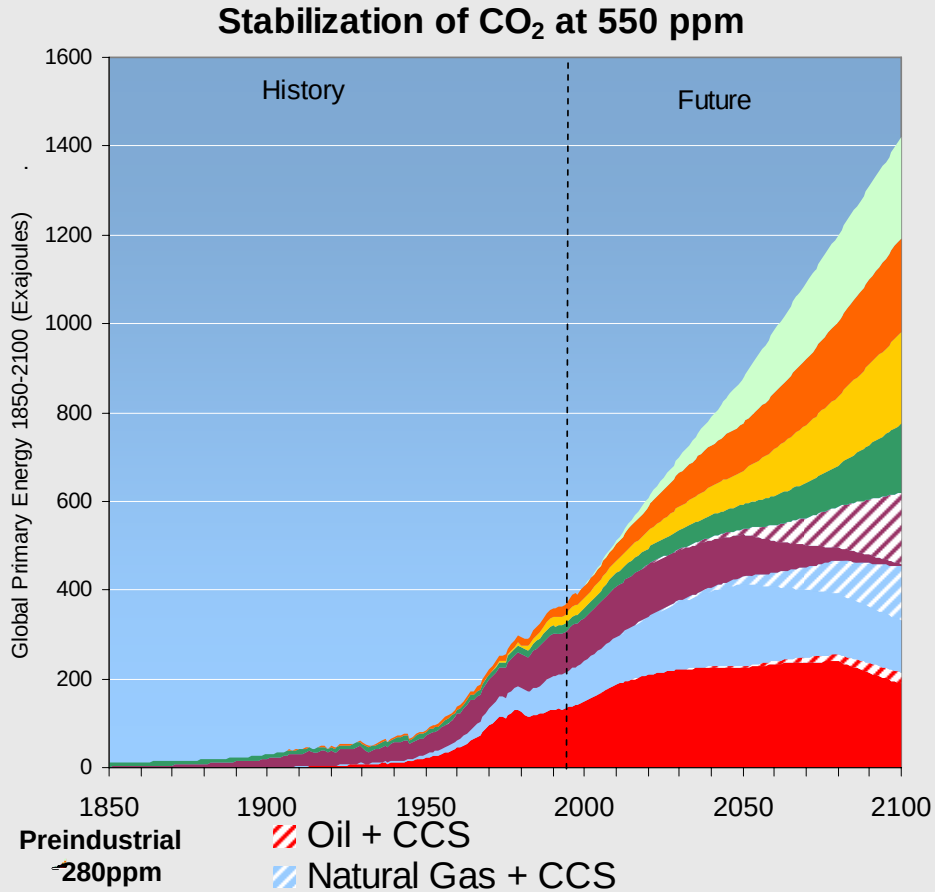
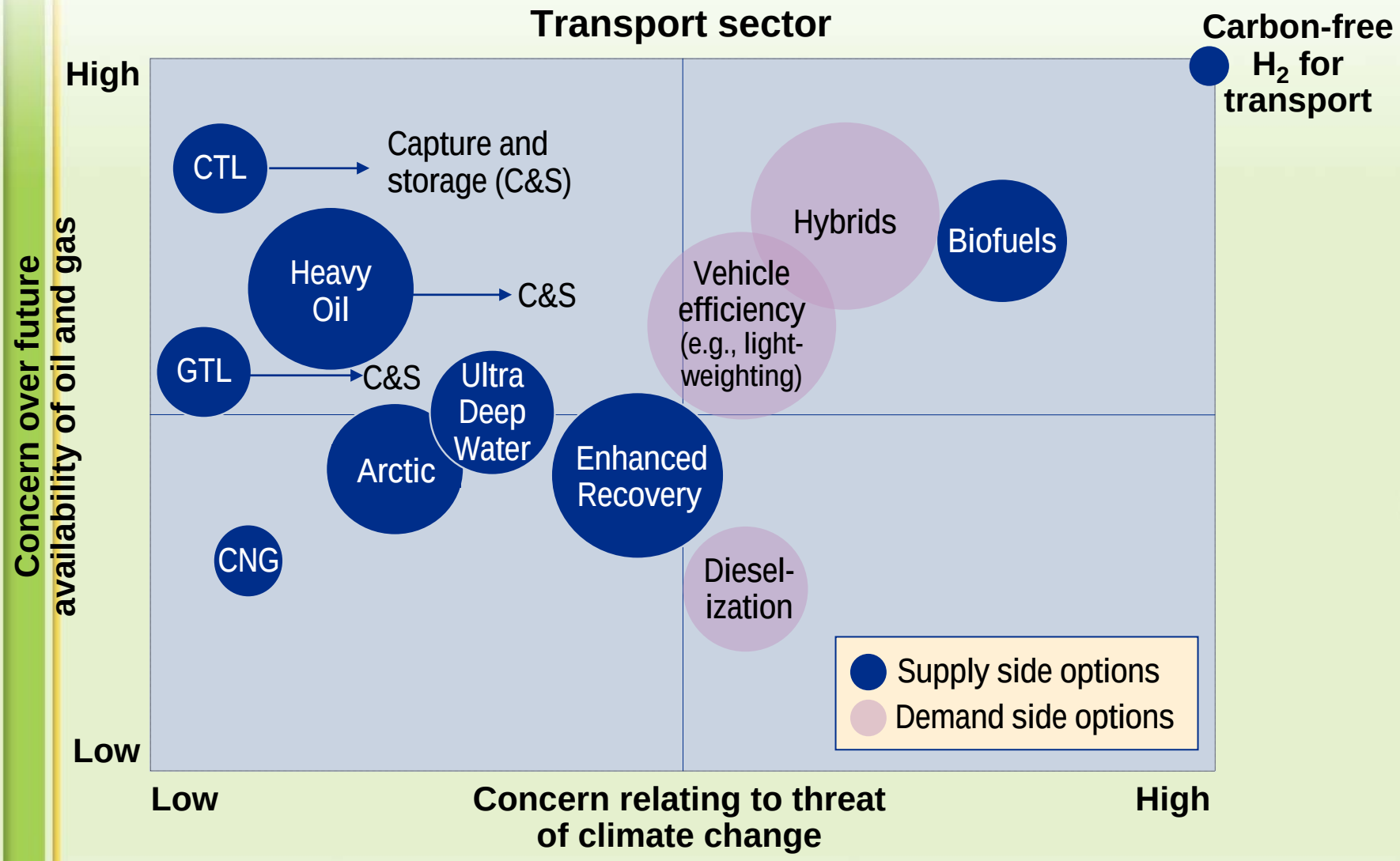
Stabilization of CO_2 concentrations means fundamental change to the global energy system

Source: Jae Edmonds





Technology options for transportation



Source: Steve Koonin, BP

Decreasing U.S. petroleum consumption

Congress: The "30 by 30" goal

- Replace 30% of gas and diesel consumption with biofuels by 2030
- Requires approximately 1B dry tons of biomass for 60B gal using current technology
- "Billion Ton Study" – there is enough biomass in the US

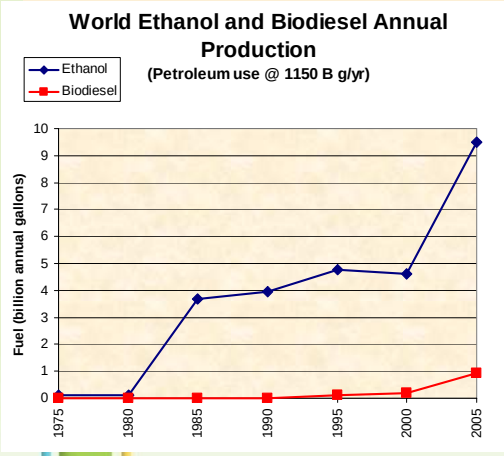
State of the Union 2007: The "20 in 10" goal

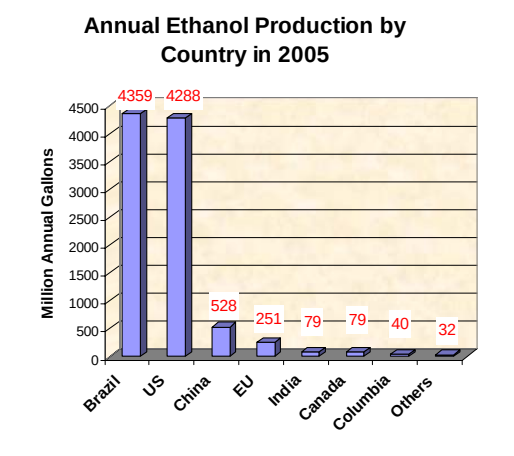
- Decrease consumption by 20% in 10 years
- Grow production of renewable fuels to 35B gal/year by 2017

Upper limit of corn ethanol is around 18 billion gal per year
(National Corn Growers Association)

With capacity being built we will reach this limit within two years

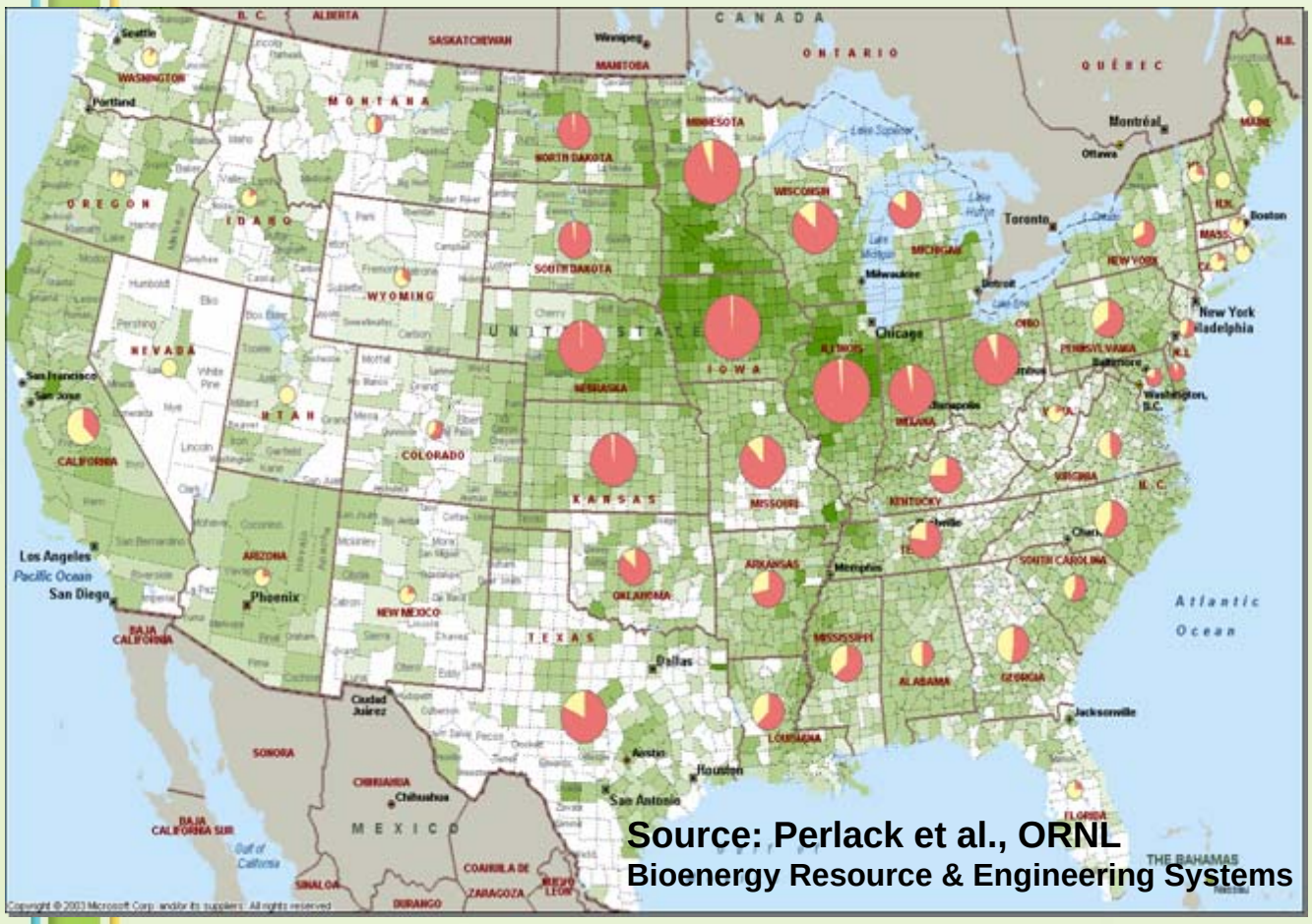
We must add cellulosic biofuels in order to meet our national goals





Potential biomass resource and refinery capacity in 2030

Forest residues (all), crop residues, switchgrass



Data do not include pulp & paper assets in the Southeast

The Southeast and Midwest will be the sources for US biomass

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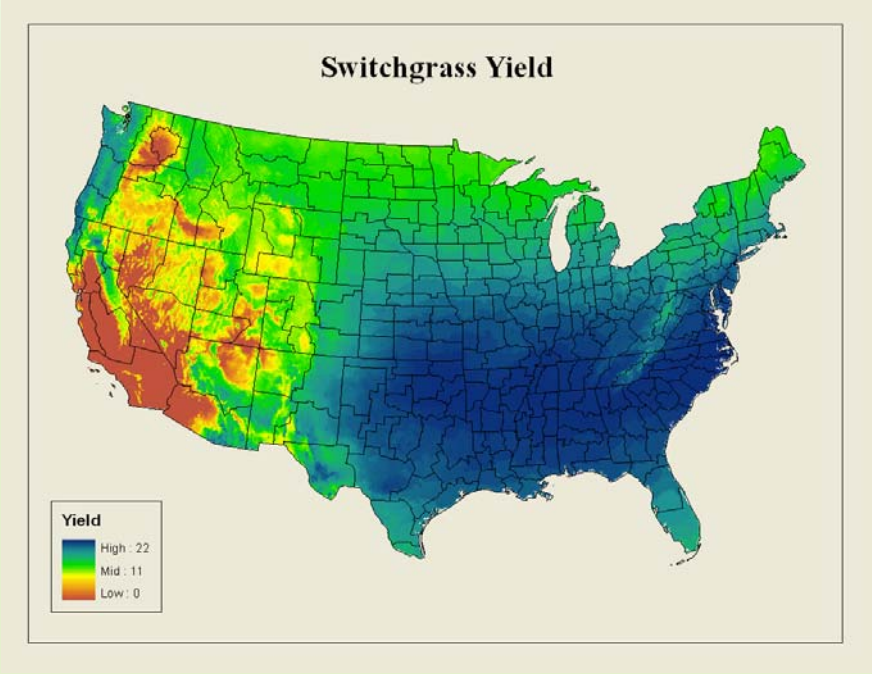
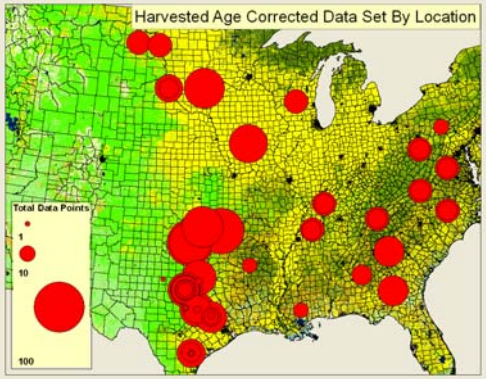
Billion-ton follow-up

Source: Bob Perlack et al, ORNL
Bioenergy Resource & Engineering Systems



- Developed new fine-scaled estimates of potential switchgrass productivity
  - **Extend to woody crops (with USDA Forest Service)**



Multiplicative model estimates yield as the product of estimated maximum yield, Y_{max} and the fractional reduction due to each limiting variable, temperature (T) and precipitation (P)

$$Yield = Y_{max} \frac{Y(T)}{Y_{max}(T)} \frac{Y(P)}{Y_{max}(P)}$$

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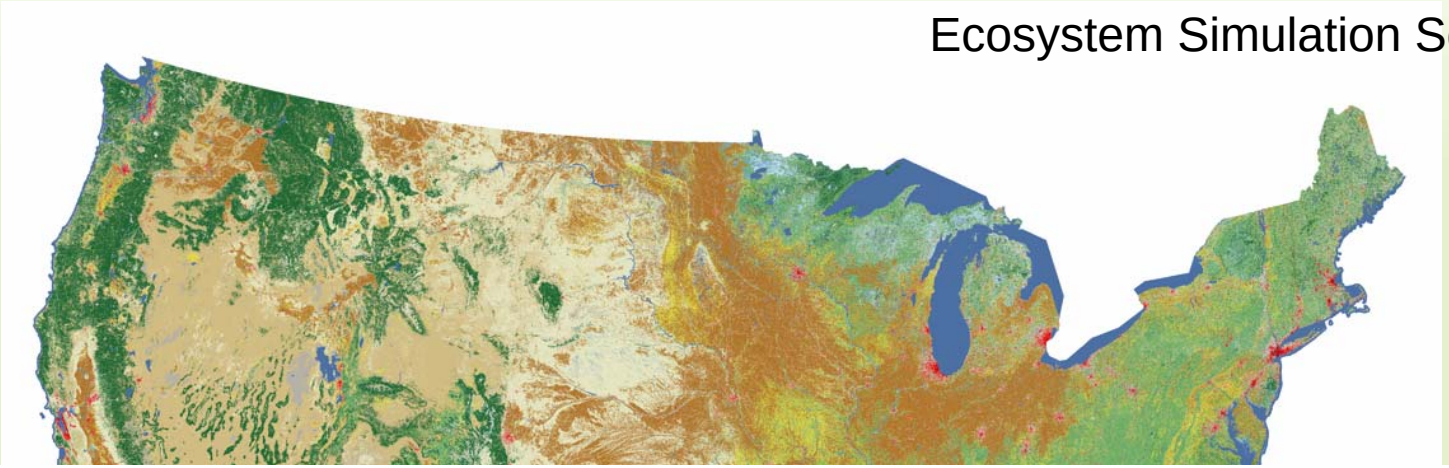
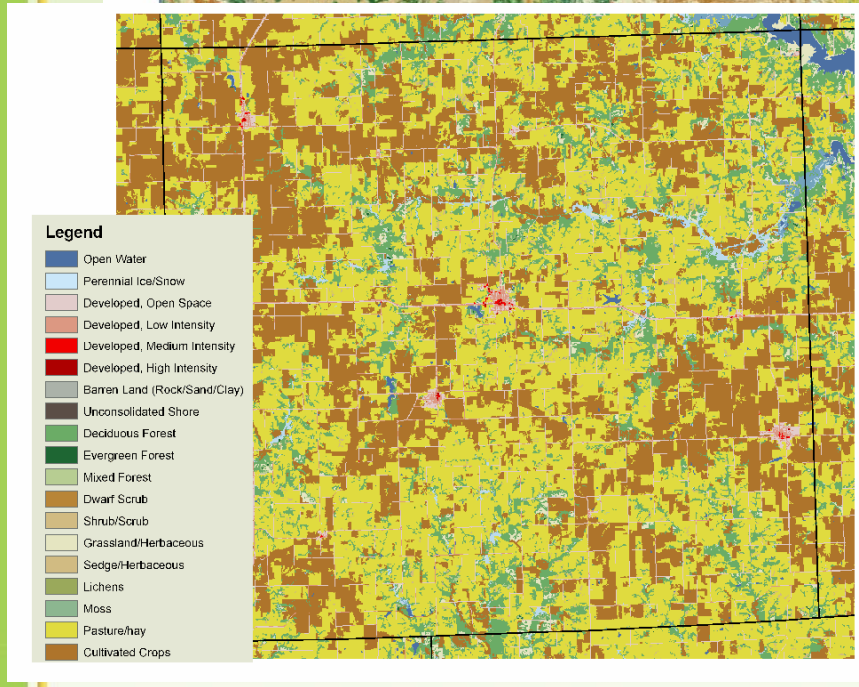
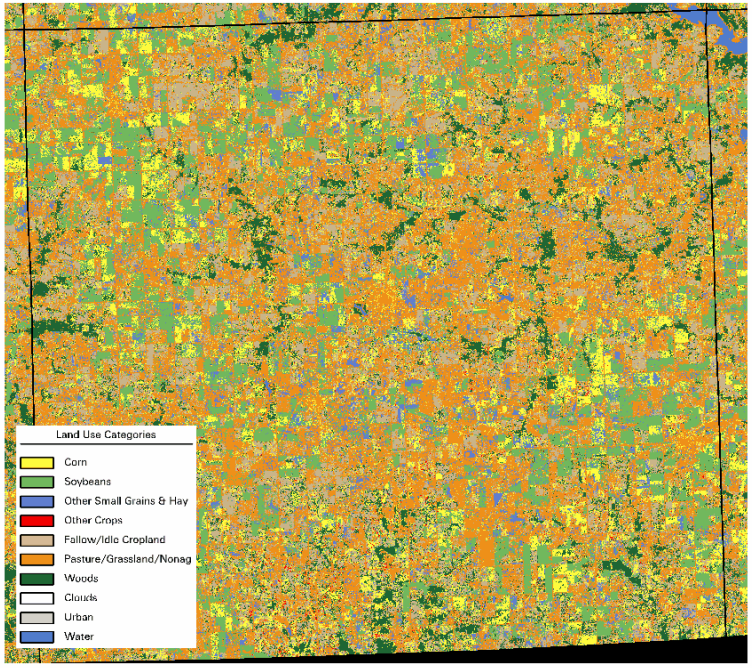
Combining National Land Cover Data with the Cropland Data Layer

Source: Tris West et al, ORNL Ecosystem Simulation Science

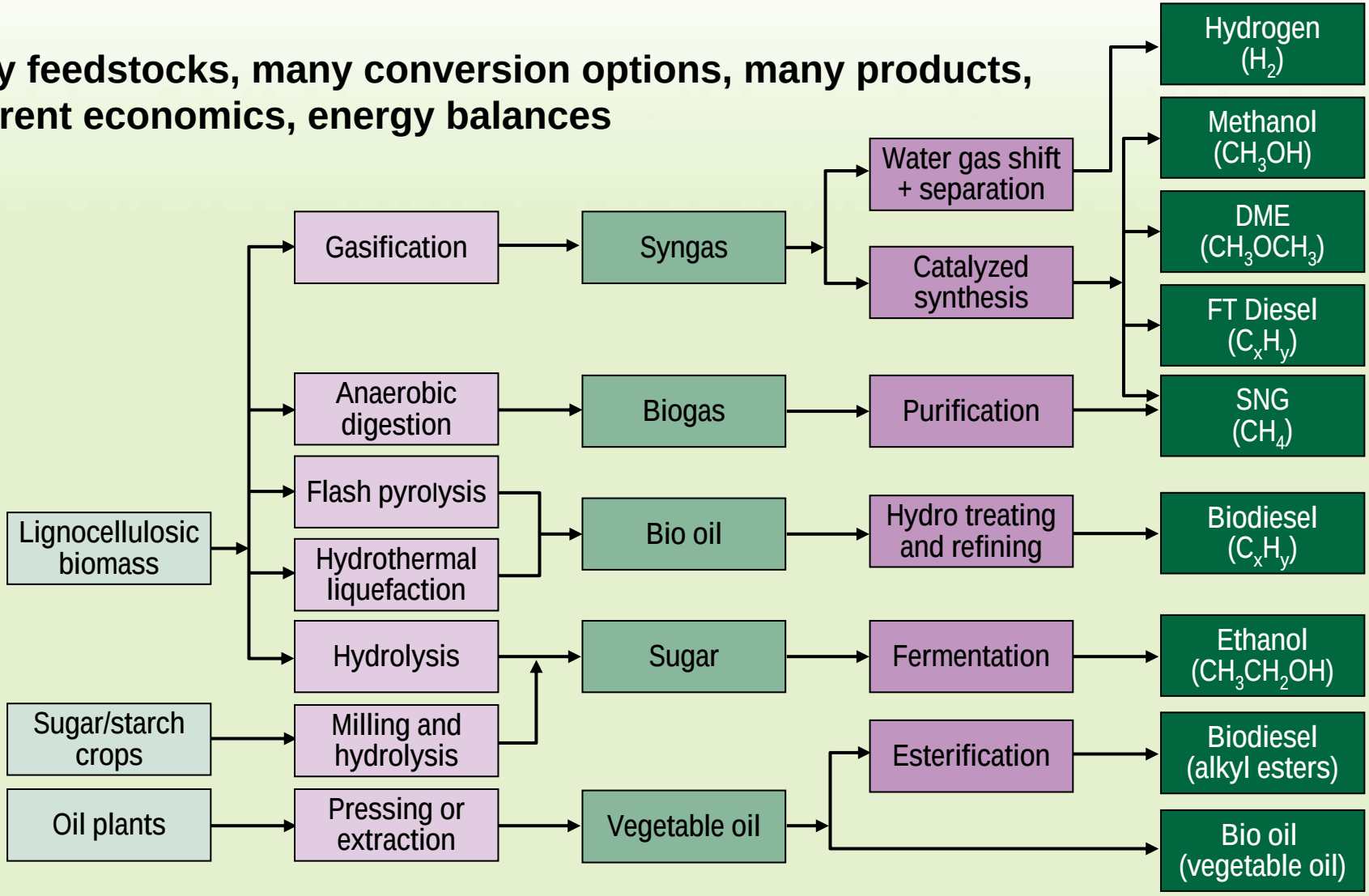






Conversion routes to biofuels

Many feedstocks, many conversion options, many products, different economics, energy balances



Source: Carlo N. Hamelinck, "Outlook for Advanced Biofuels," PhD Thesis, Utrecht University, The Netherlands, 2004

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ORNL leads one of three DOE Bioenergy Research Centers

- **Funded for $125M over 5 years**
  - **Awarded June 26**
- **Start September 07**
- **Interface with Tennessee Biofuels Initiative**
- **Two other centers at**
  - **U Wisconsin**
  - **www.wisconsinbioenergy.com**
  - **LBNL**
  - **jbei.lbl.gov**

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http://www.bioenergycenter.org

The BESC team has been assembled to overcome biomass recalcitrance

Joint Institute for Biological Sciences

Alternative Fuels User Facility

Complex Carbohydrate Research Center

- Oak Ridge National Laboratory
- University of Georgia
- University of Tennessee
- National Renewable Energy Laboratory
- Georgia Tech
- Samuel Roberts Noble Foundation
- Dartmouth
- ArborGen
- Verenium (formerly Diversa)
- Mascoma
- Individuals from U California-Riverside, Cornell, Washington State, U Minnesota, NCSU, Brookhaven National Laboratory, Virginia Tech

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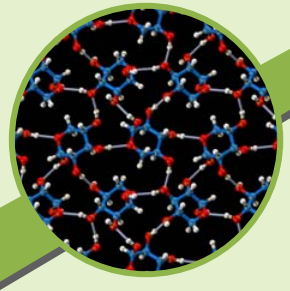
The fundamental science of biomass recalcitrance is poorly understood

Overcoming recalcitrance is the single coherent overarching theme for the BESC

Recalcitrance: Resistance to breakdown into sugars

Cellulosic biomass



Sugars

Fuel(s)

- A large-scale, integrated, interdisciplinary approach is needed to overcome this problem
  - Current research efforts are limited in scope
  - BESC will launch a broad and comprehensive attack on a scale well beyond any efforts to date
- Without advances, a cellulosic biofuels industry is unlikely to emerge
- Knowledge gained will benefit other biofuels and biofeedstocks

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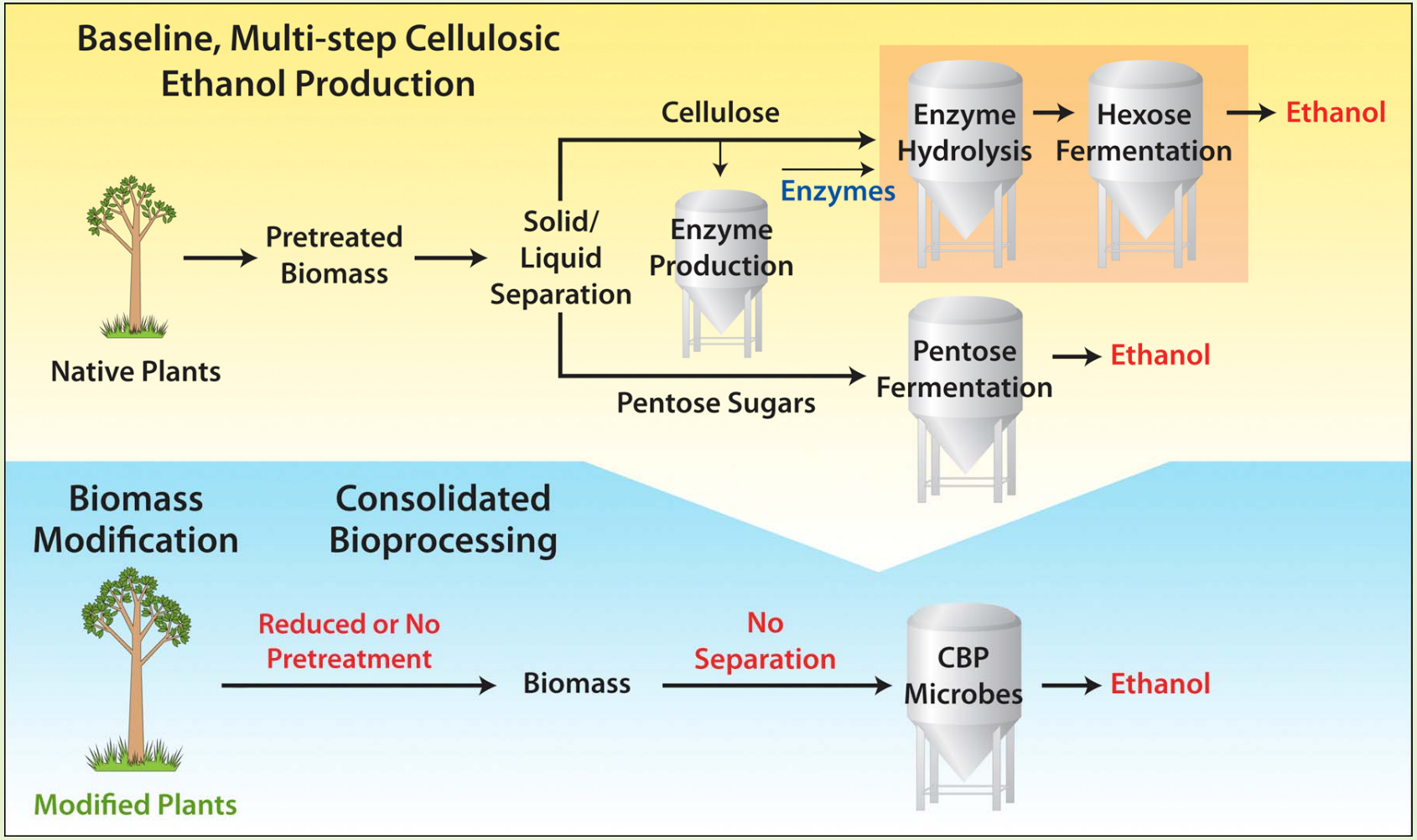
BESC will revolutionize how biomass is processed within five years



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BESC has well-defined objectives

Revolutionize the processing of biomass within 5 years

- **Improve overall yields**
- **Simplify operations through consolidated bioprocessing (CBP)**
- **Decrease (or eliminate) the need for costly chemical pretreatment**

Apply a systems biology approach and new higher-throughput pipelines

- **Reduce recalcitrance by targeted modification of plant cell wall composition and structures**
- **Develop and understand single microbes or microbial consortia and their enzymes to enable CBP for low-cost cellulose hydrolysis and fermentation**
- **Provide a synergistic combination of modified plants and CBP for even more cost-effective biofuel production**

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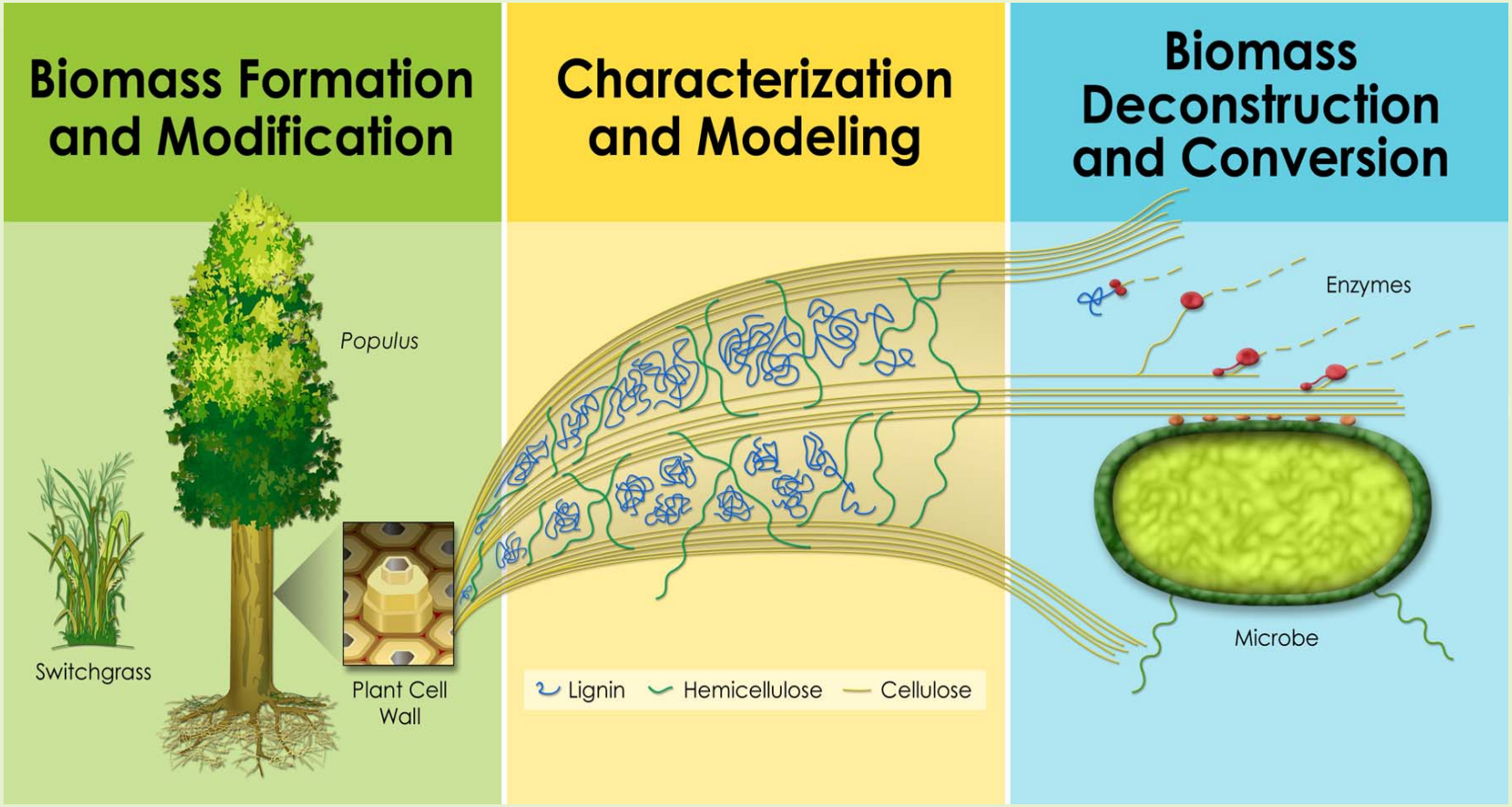
Three linked scientific focus areas will enable BESC to understand and overcome biomass recalcitrance



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BESC integrates three key science focus areas

Biomass formation and modification	Characterization and modeling	Biomass deconstruction and conversion
• What gene products control cell wall structure, composition, and recalcitrance? • How will changes in cell wall structure and composition affect plant productivity, pest resistance, and/or sustainability?	• What structural and compositional elements contribute to recalcitrance? • Can new analytical methods, systems biology data, and computational models enable predictive simulation of lignocellulose formation and deconstruction?	• What limits the rate of biomass deconstruction, and how can these limits be overcome by altered biocatalysts? • Will the combination of altered cell walls with better conversion offer a breakthrough?
Challenge: Identify genes that control biomass production and cell wall synthesis	Challenge: Understand the complexity of plant cell wall structure and its relationship to recalcitrance	Challenge: Improve deconstruction rates and understand how microbes and enzymes attack biomass substrates

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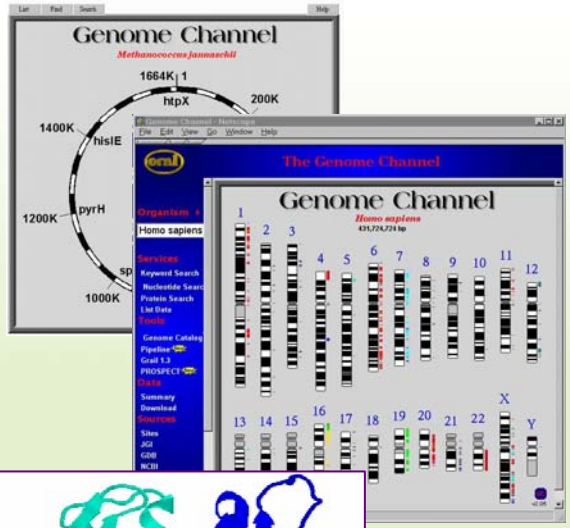
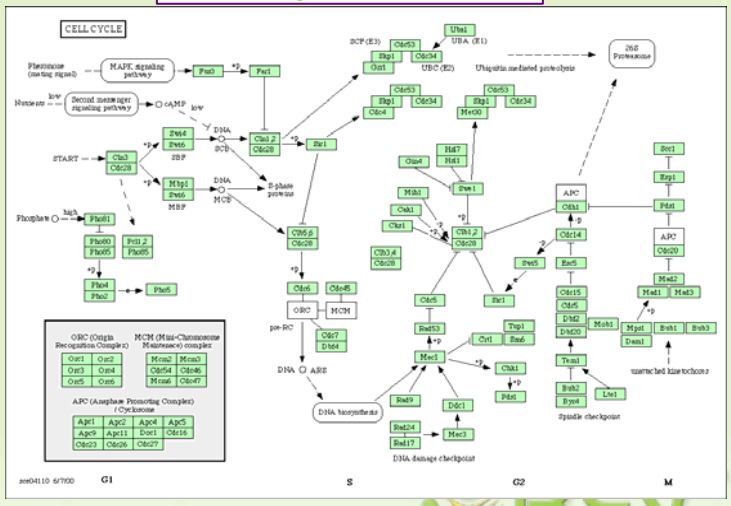
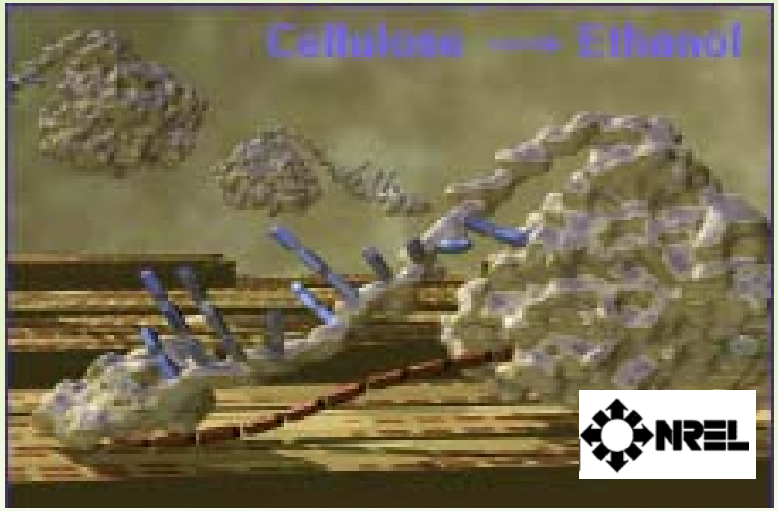
Computational Biology

- Annotation, DNA sequence analysis, gene finding, regulatory regions, comparative analyses - plants and microbes
- Systems analysis of mRNA and protein expression patterns
- Metabolic and regulatory network reconstruction in plants and microbes
- Image analysis and reconstruction software for 3-D tomography or confocal, cryo-EM
- Protein structure prediction and docking calculation
- Protein complex molecular dynamics







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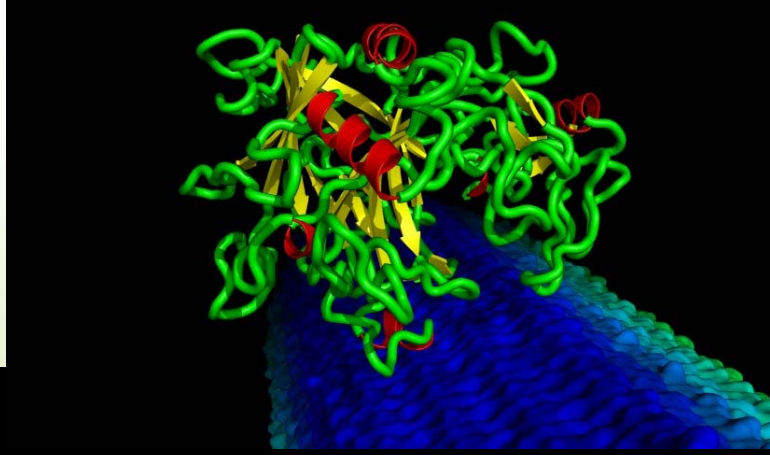
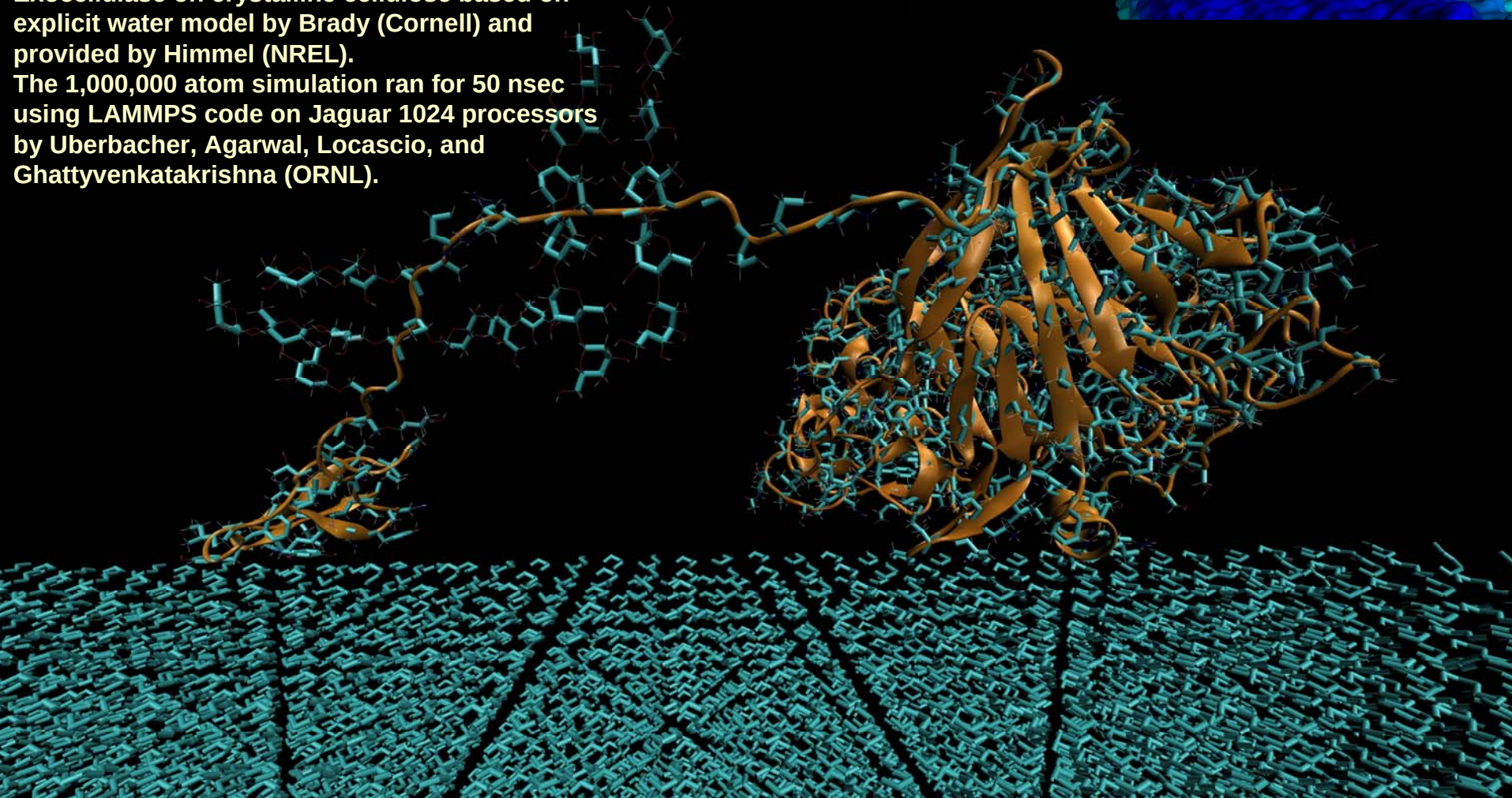
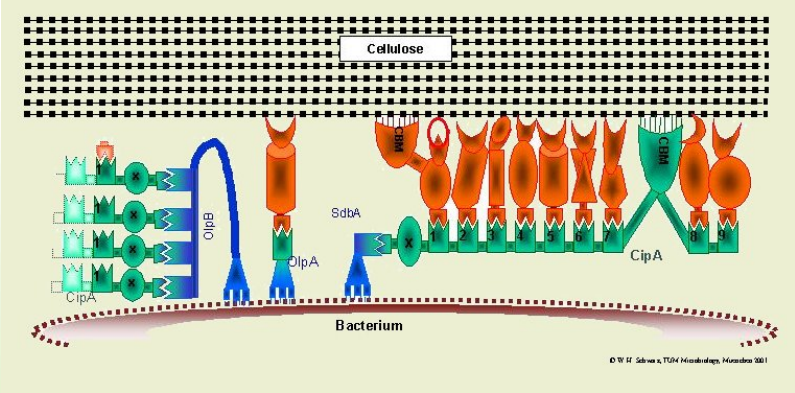
Ultra-scale modeling and simulation of biological systems



Exocellulase on crystalline cellulose based on explicit water model by Brady (Cornell) and provided by Himmel (NREL).
The 1,000,000 atom simulation ran for 50 nsec using LAMMPS code on Jaguar 1024 processors by Uberbacher, Agarwal, Locascio, and Ghattyvenkatakrishna (ORNL).



Ultra-scale modeling challenges in BESC

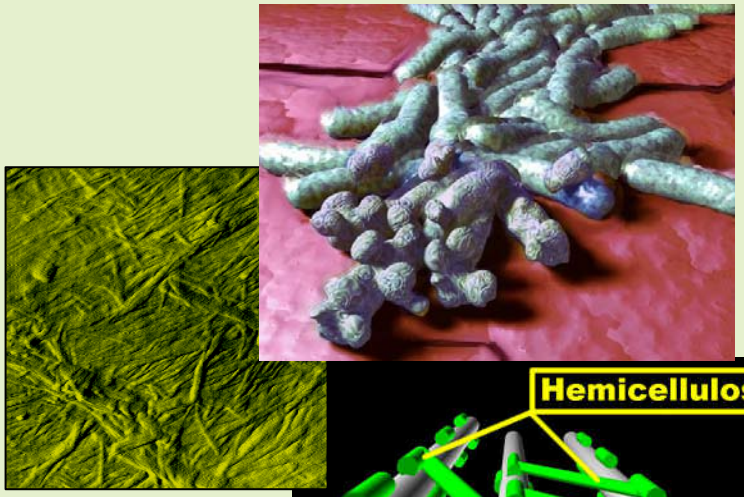


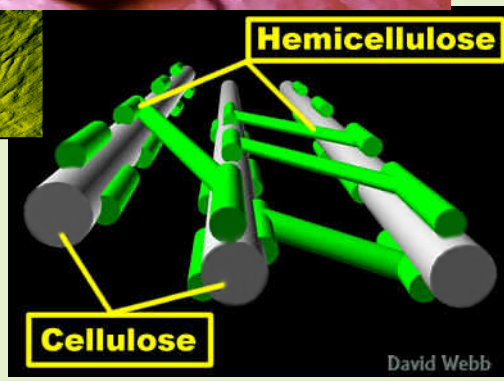
Larger scale (e.g. cellulosomes) - Increase in scale to 10's of millions of atoms

Millisecond timeframes

Multiscale simulation methods and force fields for systems of 100 million atoms scale – microbial and plant cell wall structures and cellulosomes

New force fields based on neutron dynamical measurements integrated with computational molecular simulation





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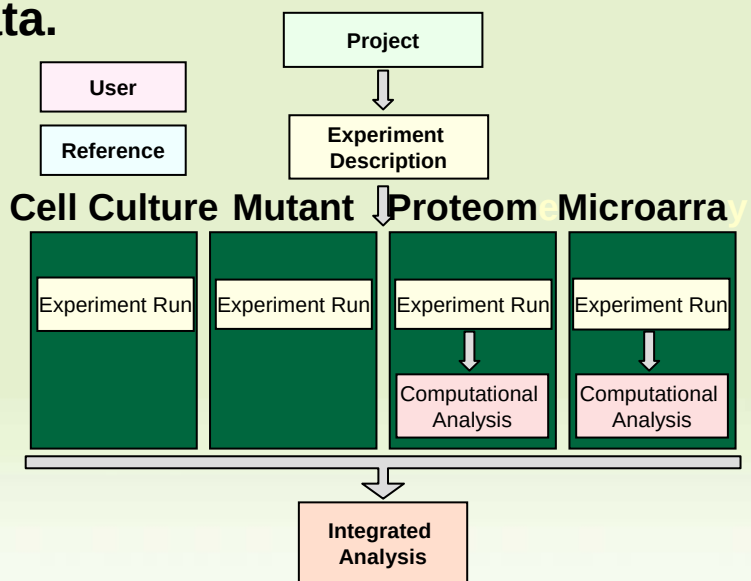
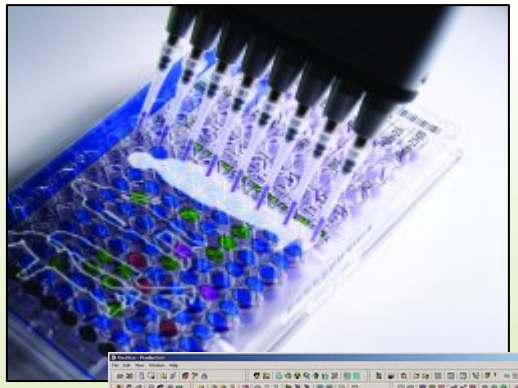
Data Management and Integration

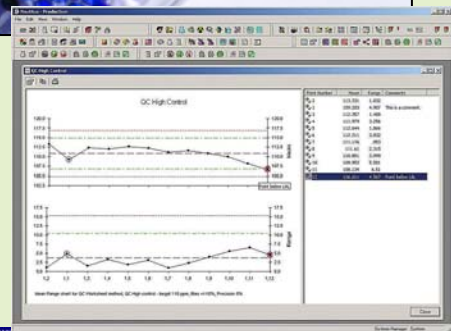
Laboratory Information Management System for tracking samples, procedures, data, IP, models

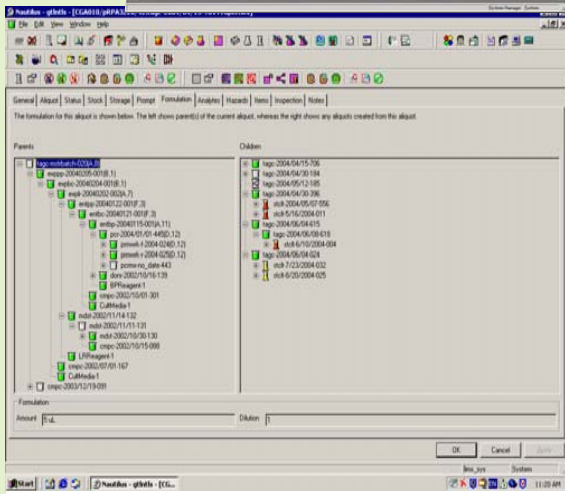
Lab instrument / user input interfaces to LIMS for data input and tracking

Systems knowledge base with data and information about key plants and microbes in the Center, metabolic, regulatory and signaling maps, with links to primary genome sequence annotation and underlying experimental data.









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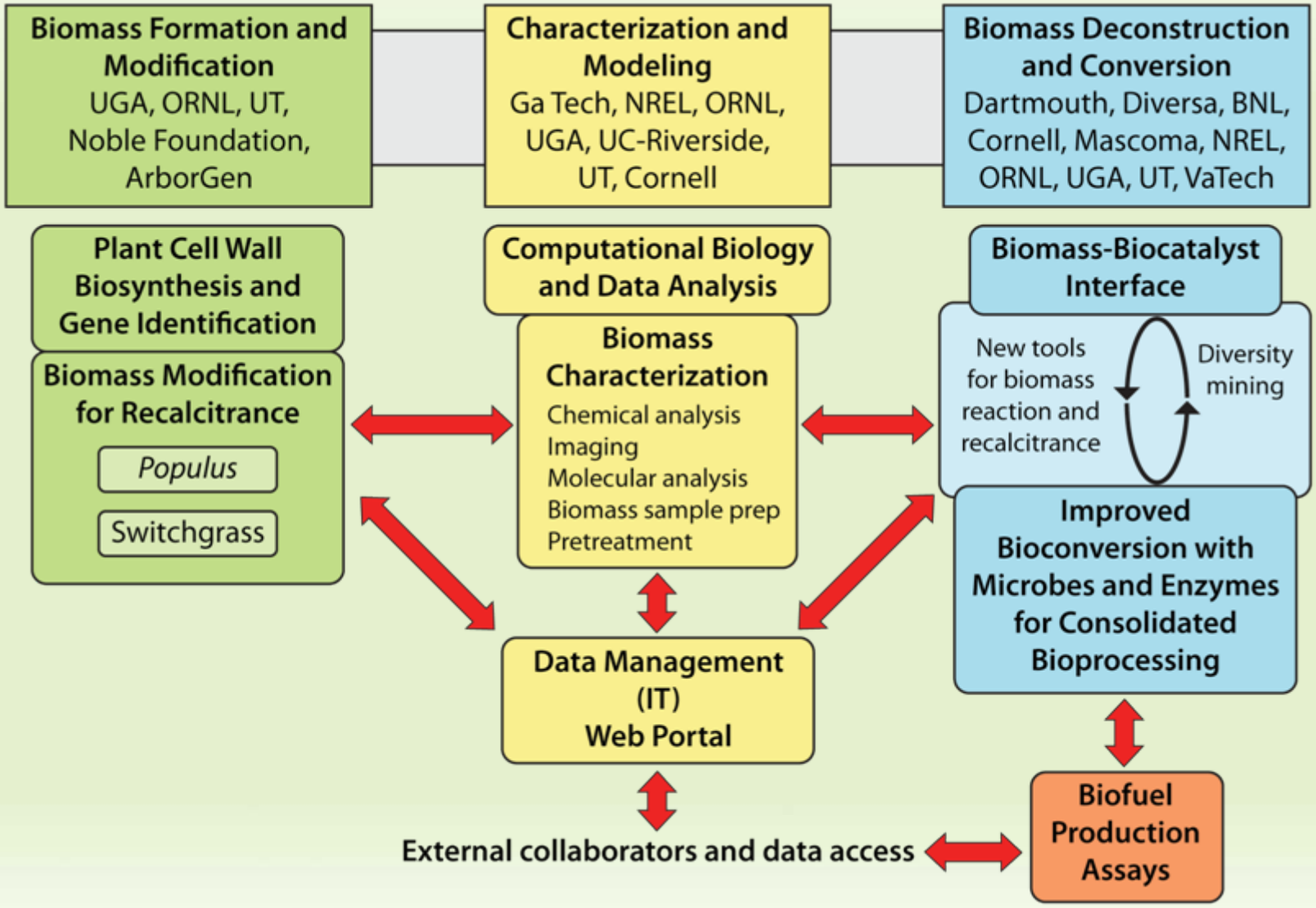
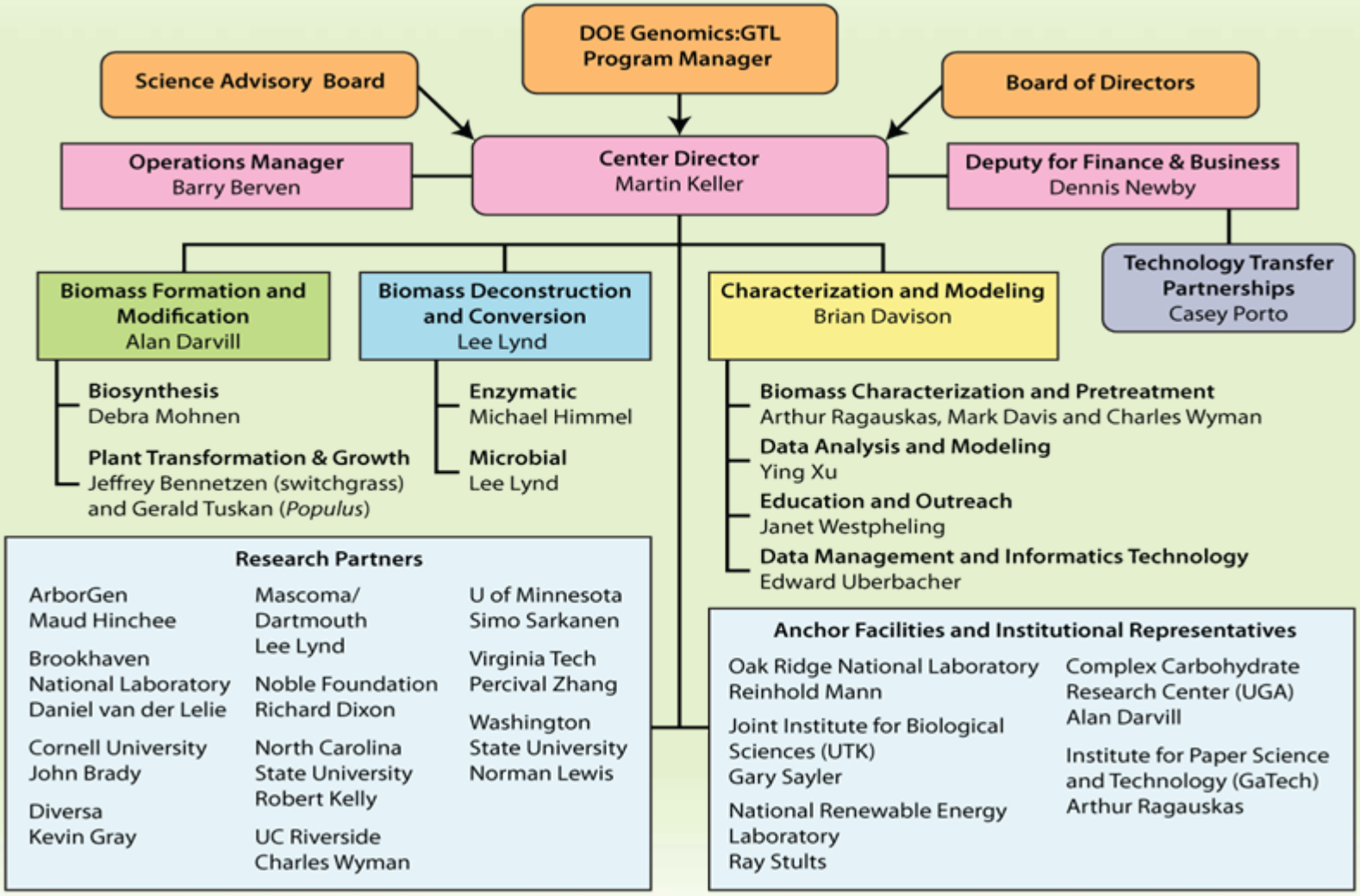
BESC – a highly integrated cutting-edge research team



A functional management structure integrates BESC activities and objectives with clear lines of authority



BESC leverages substantial firm commitments and investments

- State of Tennessee, through UT: >$24.6M
  - JIBS construction: $11.6M
  - Research equipment: $3M
  - Joint UT-ORNL research: $10M
  - 3 Governor's Chairs: $3M–$5M
- State of Tennessee: $48M
  - $40M for 5M-gal/year pilot switchgrass-to-ethanol facility, located <40 miles from ORNL, to be operational in 2009
  - $8M in agricultural price supports
- Georgia Research Alliance: $6M
  - $3M for equipment,
  - $1.5M for two Eminent Scholar hires (matched by $1.5M from UGa and Georgia Tech)
- Virginia Tech: $0.5M in cost share support
- Oklahoma Bioenergy Center
  - Update to Governor Henry's letter
  - >$10M at the Noble Foundation as part of this $40M center with University of Oklahoma and Oklahoma State

Total: More than $90M

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BESC's distinctive strengths

- **One coherent focused theme: Biomass recalcitrance**
- **Positioned to attack the most important current barrier to the emergence of a cellulosic biofuels industry**
- **The best team and management for revolutionary advances to overcome recalcitrance**

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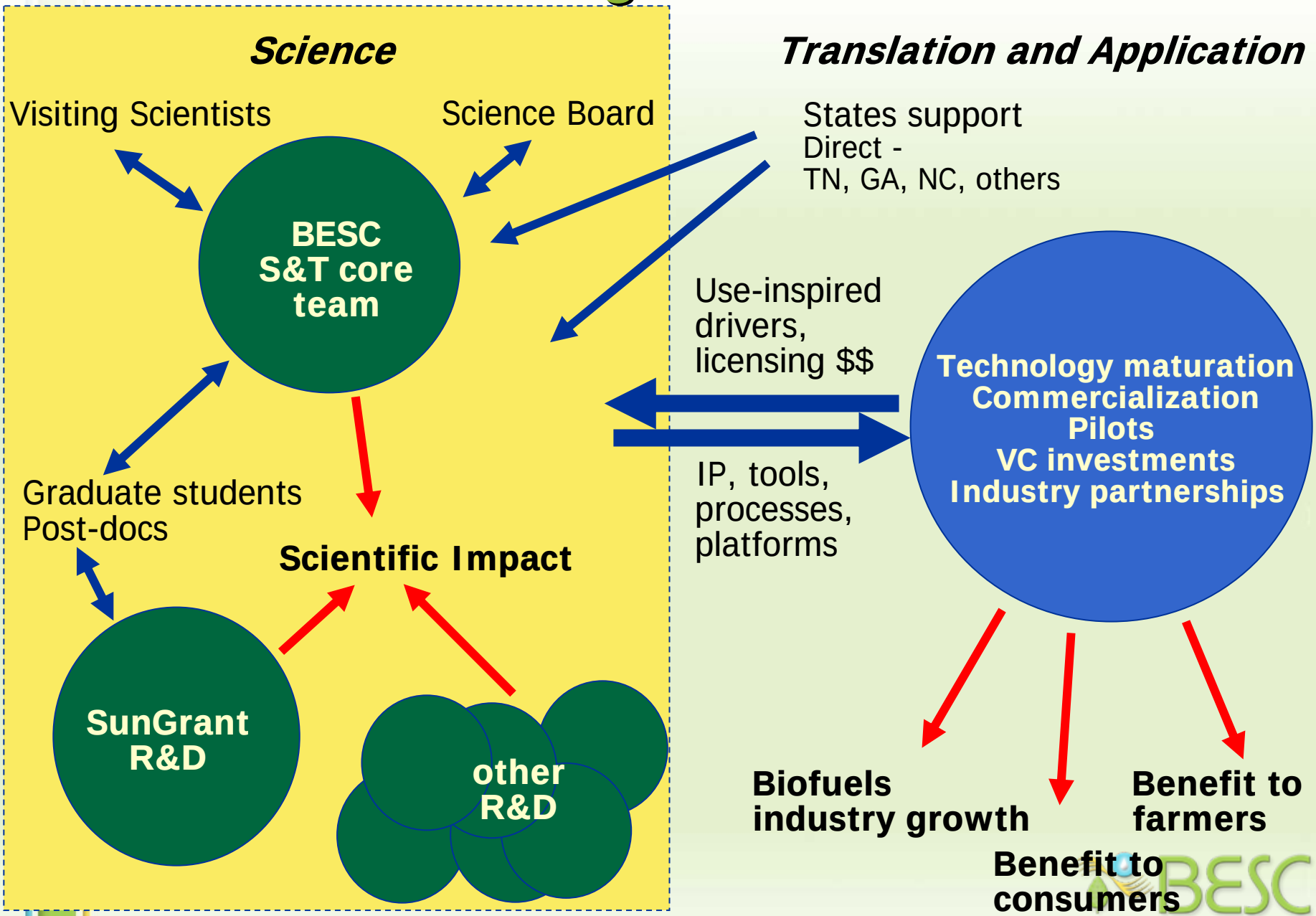
BESC larger context



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