

## NREL Carbon Metabolism Modeling Intends to Make Biofuels Engineering Routine and Reliable

NREL's early demonstration of "systems biochemistry" links traditional and emerging biochemistry with modern computing and the mathematics of complex systems.

National Renewable Energy Laboratory (NREL) scientists, supported by the Department of Energy (DOE) Scientific Discovery through Advanced Computing (SciDAC) Program, have assembled and simulated a model of key eukaryotic carbon metabolism that intends to move biochemical simulations into new realms of chemical fidelity.

Achieving truly predictive metabolic engineering requires moving beyond small canonical models to realistic, large-scale, dynamic systems that describe cellular biochemical networks.

NREL researchers assembled a multi-compartmental metabolic model comprising 149 compounds, 65 enzymes, 688 parameters, and 114 reactions that describe the key pathways of glycolysis, tricarboxylic acid cycle, reductive pentose phosphate, oxidative phosphorylation, starch degradation, and fermentation, including the full complexity of kinetic equations.

Ongoing high-performance simulation and analysis of this model using NREL's supercomputing capability—including a parallel software simulation and optimization suite developed at NREL under the same DOE program—will yield a new understanding of how biochemical systems respond to physical changes in conditions.

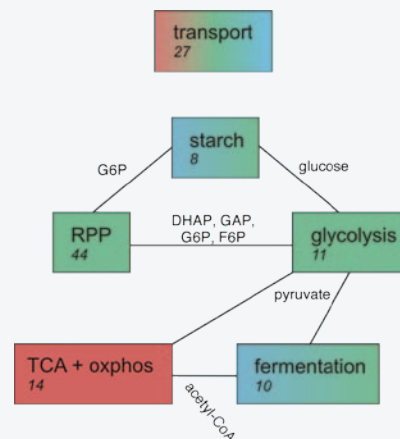
NREL envisions this work to be an early demonstration of systems biochemistry that can join together traditional and emerging biochemistry with modern computing and the mathematics of complex systems.

As our understanding of cellular metabolism advances through partnership among experiment, computation, and theory, cellular design will become as routine and reliable as automobile design is today.

**References:** Lunacek M, Graf P, Nag A, Chang CH, Kim K, Seibert M. 2011. Modeling the Parallel Performance of CMA-ES. J. Phys. Conf. Ser., in press.

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### Key Research Results

#### Achievement

New simulation model coupled with NREL's supercomputer advances biochemical modeling reliability.

#### Key Result

NREL created the largest and most detailed model to date related to central carbon flow.

#### Potential Impact

This research will lead to a greater understanding of biochemical dynamics with applications to metabolic engineering and production of biofuels.