BioLEGO: From Biomass To Product
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Background

Efficient and sustainable conversion of biomass into valuable products is a major challenge for bioengineering.

The composition of the available feedstock biomass and the ability of microorganisms to efficiently ferment it are two most critical factors influencing the process efficiency.

Even in the two-organism fermentation system, an analysis of many promising scenarios may require solution of millions of optimization tasks.

Simulations and computer-assisted optimization are valuable tools for fermentation processes designers.

We present BioLEGO, a Microsoft Azure Cloud-based framework, delivering these heavy calculations to unskilled users.

Modeling

Flux Balance Analysis (FBA) framework

The reaction stoichiometry in a metabolic model is represented by matrix $S$, wherein $S_{rm}$ corresponds to stoichiometric coefficient of metabolite $m$ in the reaction $r$.

The vector of metabolic fluxes that are carried by the model reactions, normally denoted as $v$, is constrained both by mass-balance and by maximal/minimal feasible fluxes $v^{\max}$ and $v^{\min}$.

Modular Approach – Single Module

Modular Approach – Combining Modules

Formulation of Optimization problem

Experimental Validation

Use Case

Analyzing 6.6M knockouts in two-step process

Heatmap of knockout performances

GOrilla analysis
(Enriched Functionality in results of S. cerevisiae)