DFBALab – MATLAB Code for Dynamic Flux Balance Analysis
Technology #18411

Applications

The inventors present a dynamic flux balance analysis (DFBA) simulator in MATLAB that performs fast, reliable, and flexible simulations of genome-scale metabolic processes. The presented DFBALab framework has application to advanced biofuel production as well as to other bioprocess engineering industries.

Problem Addressed

Dynamic flux balance analysis (DFBA) provides a quantitative modeling framework used to simulate dynamic biochemical processes. Typical dFBA models use solutions of linear programs (LPs) to predict species concentrations. Common challenges with classic DFBA simulators involve the LPs becoming infeasible or producing non-unique solution sets. This results in failure during numerical integration and limits the reliability of simulated results.

Technology

This non-patented MATLAB-based code provides efficient and reliable simulation of genome-scale metabolic process in dynamic batch cultures. DFBALab uses lexicographic optimization to obtain unique exchange fluxes and the LP feasibility problem to generate an extended dynamic system and penalty function. These combined features result in a faster, more accurate modeling framework to simulate complex biochemical processes.

DFBALab offers a reliable, easy-to-use implementation that minimizes troubleshooting of numerical issues and facilitates focus on the analysis of simulation results. The tool uses commercial linear program solvers such as CPLEX, Gurobi, and MOSEK and is compatible with the COBRA toolbox model format.

Advantages

- Fast, reliable, and flexible community simulations
- Does not fail in presence of infeasible linear programs (LPs)
- Extended system produces a penalty function for optimization algorithms

Categories For This Invention:

Computer Sciences & Information Technology
Simulation & Modeling
Energy
Biofuels (Energy)
Intellectual Property:
Copyright Software

Inventors:
Paul Barton
Jose Gomez
Kai Hoffner

Publications:
DFBAlab: a fast and reliable MATLAB code for dynamic flux balance analysis
BMC Bioinformatics
2014, 15:409

External Links:
Process Systems Engineering Laboratory
https://yoric.mit.edu/