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In This Issue

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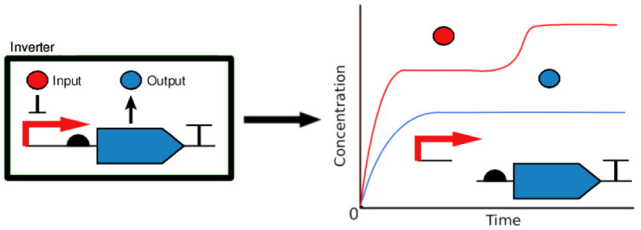
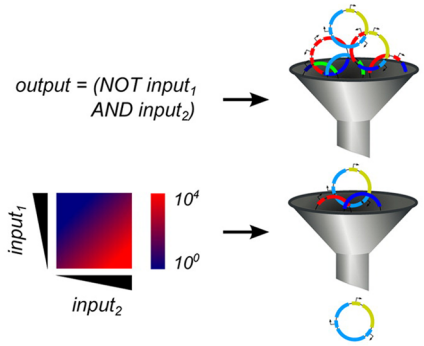
GENERATING SYSTEMS BIOLOGY MARKUP LANGUAGE MODELS



In this paper, Roehner *et al.* (DOI: 10.1021/sb5003289) describe a methodology for generating Systems Biology Markup Language (SBML) models from genetic designs written in a recently published proposal for the next version of the Synthetic Biology Open Language (SBOL). This methodology has been implemented in the authors' genetic design automation (GDA) software tool, iBioSim, and can be used to supplement repositories of qualitative genetic circuit designs with quantitative biochemical models. In this way, when performing other design tasks in iBioSim that yield a composite genetic circuit design, users are guaranteed to have a composite model that they can simulate to verify the design's theoretical function.

In a broader sense, GDA tools for model generation are useful because they can enable faster and more accurate creation of testable models that conform to genetic designs containing different types of data, such as genetic sequences, regulatory networks, and experimental measurements. In addition, by generating models written in standard modeling languages and annotating them with metadata, these tools can facilitate interdisciplinary collaboration and comparison of models generated by different research groups.

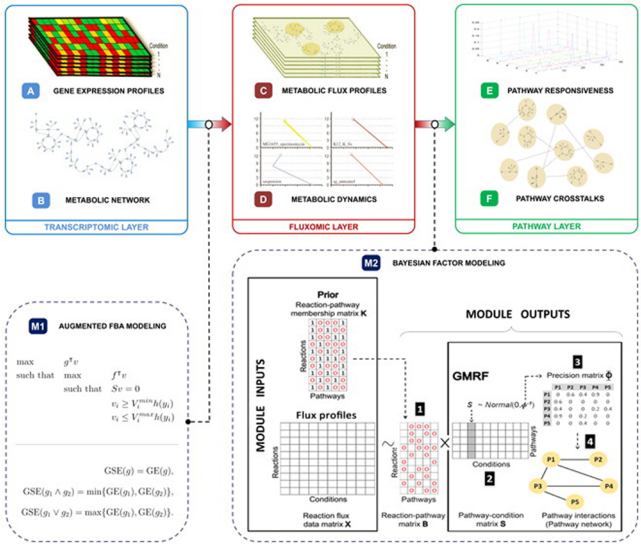
FAST AND ACCURATE CIRCUIT DESIGN AUTOMATION THROUGH HIERARCHICAL MODEL SWITCHING



In the field of computer-aided biological design, characterized part libraries, accurate models and optimal design parameters are essential for producing reliable designs. While significant progress has been made over the years, limitations such as scalability, optimality and biological accuracy still persist. Here, Huynh and Tagkopoulos (DOI: 10.1021/sb500339k) describe a two-tier methodology for selecting the optimal design, in a fast and accurate manner, given a part library and input/output specifications.

The authors first use a simple model of low computational complexity to predict circuit behavior and assess candidate circuit branches through branch-and-bound methods. Then, a complex, nonlinear circuit model is used for a fine-grained search of the reduced solution space, resulting in more accurate results.

A HYBRID OF METABOLIC FLUX ANALYSIS AND BAYESIAN FACTOR MODELING FOR MULTIOMIC TEMPORAL PATHWAY ACTIVATION



The increasing availability of multiomic data enables the mapping of cellular processes at the mRNA, protein, and metabolite levels. In this study, Angione *et al.* (DOI: 10.1021/sb5003407) develop a novel method that exploits these multiomics data to study the response of *Escherichia coli* to a variety of environmental conditions, and over time. This method integrates an augmented flux-balance analysis framework with Bayesian factor modeling, with the aim of determining interactions between biological pathways and building pathway activation profiles from different experimental conditions.

Using gene expression data, obtained under various growth conditions, the authors were able to detect pathway cross-correlations and predict metabolic pathway activation profiles. This ability to predict the functionality of particular groups of reactions is very useful in the analysis of omics data and of great interest to the field of metabolic engineering.

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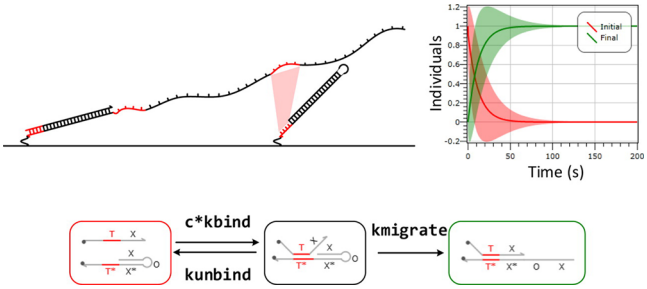
PROBABILISTIC ANALYSIS OF LOCALIZED DNA HYBRIDIZATION CIRCUITS



DNA is programmable biological material that naturally interfaces with biomolecular components and has great potential for applications in biofabrication and smart therapeutics. While recent work has demonstrated the computational potential of DNA, a major drawback of DNA-based systems has been the slow speed of computation. One approach to overcoming this is to colocalize interacting molecules on a fixed substrate, mimicking natural biological systems that use clustering and compartmentalization to increase the effective rate constants of biomolecular interactions. Here, Dalchau *et al.* (DOI: 10.1021/acssynbio.5b00044) propose designs for localized circuits involving DNA molecules that interact *via* hybridization reactions, and demonstrate how to encode and analyze these localized circuits using the Visual DSD software.

The authors applied their designs and analysis methods to localized implementations of Boolean logic and demonstrated that localized DNA hybridization circuits have increased speed, precision, modularity, and scalability. They further show that, with appropriate design strategies, localized circuits can retain these advantages in the presence of unintended interferences between strands.

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