

Software package for analysis of regulatory circuits of bacterial metabolic pathways by mathematical modeling methods

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Motivation and Aim: Today there are many tools and libraries available within engineering modeling environments that can be used to create mathematical models of the regulatory circuits of bacterial metabolic pathways. However, such models should be created using approaches and standards recognized by the scientific community. Such approach is the “Elementary Subsystems” approach, on which DSL tools and model representation standards SBML, SBGN, CellML, etc. are based. In the study, we present a working algorithm and its software implementation for reconstructing and analyzing large regulatory circuits, commonly arising in automatic generation problems with dozens/hundreds of subsystems.

Methods and Algorithms: The algorithm is implemented in Python programming language as package of Jupyter Notebooks. The basico library (basico.readthedocs.io) is used to build the model. Computational experiments are performed in the Copasi tool (copasi.org). The final model is implemented in SBML standard (sbml.org).

Results: Nowadays, information on regulatory relationships is built based on automated tools for whole-genome analysis and we obtain dozens/hundreds of nodes in regulatory circuits. The transition in reconstruction from such large-scale regulatory contours to their mathematical models within existing tools providing WYSIWYG approaches (as Copasi, CellDesigner, ECell) of model building is a rather labor intensive process. The developed software package provides a prepared set of steps that automate this transition: preparation of elementary subsystems, their placement in the compartment structure, generation of a combined mathematical model (export in SBML standard) and computational experiments. Setting additional features in the circuit elements annotation is the necessary step of customizing data post-processing methods for summary charts and simulation results visualization.

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