AUTOMATIC GENERATION AND NUMERICAL ANALYSIS OF MATHEMATICAL MODELS FOR MOLECULAR-GENETIC OBJECTS IN AN INTEGRATED SYSTEM OF MGS-GENERATOR AND STEP+ MODULES

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Motivation and Aim: Mathematical models allow us to naturally integrate the multi-scaled experimental data and analyze the cause-effect relationship between the molecular structure, dynamics and phenotypic features of living systems in terms of the common conceptual scheme. The increasing volume of the accumulated data stimulates the development of computer technologies for their processing, storage and analysis. That is why the development of computer tools allowing one to reconstruct and analyze mathematical models for molecular-genetic objects is one of the key problems in the era of systems biology.

Methods and Algorithms: The paper describes a new computer system for generating and analyzing mathematical models of molecular-genetic objects, based on the integration of two program modules: MGSgenerator [1] and STEP+ [2]. MGSgenerator is designed for automatic generation of mathematical models on the basis of structural and functional organization of gene networks extracted from the GeneNet database [3]. STEP+ is a tool for numerical analysis of mathematical models presented as an autonomous system of ordinary differential equations.

Results: The computer system possibilities are demonstrated by the analysis of dynamic features of two gene networks that control auxin metabolism in a shoot meristem cell for higher and lower plants [4]. Two mathematical models were automatically generated by the MGSgenerator module based on the structural and functional organization of the corresponding gene networks. The results of the numerical analysis with the STEP+ module indicate a higher stability of the stationary intracellular concentration of auxin with respect to the model parameters for higher plants as compared with the lower ones.

Conclusion: Structural and functional organization of the program modules as well as the advantages and the results of testing the computer system are discussed in this paper.

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