Database Integration for the Simulation of Metabolic Network Control

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Today, biotechnology needs new methods to make use of the existing scientific results. Referring to molecular biology, there are lots of specific databases available by the WWW, followed by already implemented methods to query and analyse the contained data. To cover the very complex procedures of metabolic networks as we try to do it in our MARGBench project, it's finally necessary to access multiple databases. In our project we use fundamentals of the federated database approach [Con97] combined with modern internet programming technology to solve this task.

Our prototype called MARGBench[1] has been developed to logically integrate distributed molecular data from different databases. The application MetabSIM, a discrete simulation environment, is a reference application to show the functionality of MARGBench. The architecture consists of the three main components BioDataServer, MargBench-Factory and MargBench-Browser. The BioDataServer is the core of the system and is connected to the component databases by specialized database adapters. The seperate adapters can be manufactured automatically by an adapter-generator for flat/semi-structured files, multiple typs of database systems and internet information systems. After processing the adapters, they can be bound to the BioDataServer at runtime. The BioDataServer manages user-defined integrated schemes. Here the user describes, which spectrum of data should be extracted from every adapter. The BioDataServer accepts SQL-statements to query the data.

The simulation environment MetabSIM has been designed to simulate metabolic networks and bases on formal languages [HM95, HS98]. In MetabSIM the discrete states of cellular compartments are expressed by mixtures of substrates. The states are called configurations. The step from one configuration to a following (derivation) is defined by a rule-set, where each rule describes a biochemical and metabolic process.

References

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