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Computer-Aided modeling of biochemical systems

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The creation of quantitative models for gene-regulatory, signaling, and metabolic networks still constitutes a demanding task. First a network of coupled reactions or processes must be assembled, requiring intensive literature study. The program KEGG translator facilitates this effort by automatically extracting pathway information from the KEGG database. To obtain a mathematical model description for simulation, kinetic equations are required for each reaction within the network. Deriving and assembling these formulas is a complicated, time-consuming, and error-prone process that requires knowledge about the structure of interactions, consistently choosing a rate law for each type of reaction, and assignment of appropriate units to all parameters. In many cases, thermodynamic dependencies between the parameters have to be taken into account. For multi compartment models, the concentration units of reacting species have to be converted into molecular amounts. The program SBML squeezer interprets the context of each individual reaction and generates kinetic equations for entire models and equips all newly created parameters with appropriate units. Furthermore, SBML squeezer ensures consistent differential equation system creation by introducing unit conversion for reacting species. In order to estimate meaningful values of the model's parameters, the application SBML simulator brings together sophisticated numerical integration methods, an exhaustive interpreter for SBML models, and a large variety of heuristic optimization procedures. The program takes quantitative time series data of all participating species as an input and fits the model to these measurement values. Finally, the model documentation tool SBML2LaTeX allows users to automatically create a comprehensive report comprising all equations and details of the model. All these programs use the data structure JSBML and provide an Application Programing Interface (API), which makes an integration of the algorithms into more complex processes possible. The usefulness of this pipeline has been demonstrated in a large-scale batch application, in which more than 142,000 models have been created and made accessible at Biomodels.net.

Biography

Andreas Dräger studied bioinformatics at the Martin Luther University Halle-Wittenberg from 2000 through 2006. During this time he worked as an intern at the Max Planck Institute Berlin and at the University of Illinois at Chicago. He then became a Ph.D. student at the Center for Bioinformatics Tuebingen (ZBIT) and could successfully obtain his doctorate in 2011. In 2010 he worked as a visiting research student at Keio University in Yokohama. The University of Tuebingen awarded his outstanding thesis with the dissertation award 2011. He has been working as a junior group leader at ZBIT, before joining Prof. Palsson's group at the UCSD in 2013.

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