Creating a Bridge between Modelica and the Systems Biology Community

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The possibility to model and simulate signalling and metabolic pathways as well as physiological processes will play an increasingly important part of drug discovery and personalized medicine. The common ambition is to replace in vivo (within a living organism) and in vitro (artificial environment outside the living organism) tests with in silico (within a computer) tests.
There are several challenges that have to be met in order to reach this goal. For instance such in silico models need to be able to combine different levels of models (body, organ, tissue, cells, and molecules) and time scales. Furthermore, one have to deal with measurement limitations where the majority of the data is qualitative and noise levels are high, the relationship between in vivo and in vitro experiments, individual differences, as well as the large amount of unstructured data.
In order to deal with these issues MathCore and Wolfram Research, together with partners, is developing new functionality in MathModelica. In this talk a few of these challenges and what we are doing to meet them will be presented, including:
i. A translator that makes it possible to import and export between the Systems Biology Mark-up Language (SBML) and the translator has been developed in order to make it possible to take advantage of the multitude of available SBML models and use these models as sub modules in the more flexible Modelica language to create larger whole-body models.
ii. A methodology to assess the physiological relevance of cellular data obtained in in vitro experimental model systems, and merge such data in an expandable and internally consistent body of knowledge for whole-body glucose homeostasis (the ability of the body to adjust its internal environment to maintain stable glucose equilibrium) based on in vivo experiments.
iii. A framework for generating, visualizing, and documenting knowledge and models of biological reaction networks automatically from a given database of biological information (based on some standardized format).
iv. How to establish the connection between the variability in population data from clinical studies to the results from in vitro experiments, in order to meet the challenge of individualizing models.