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Automated Transformation Between Modeling Languages with Different Expressiveness: Challenges and Results From a Use Case with SBML and ML-RULES

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ABSTRACT

Automated transformation between modeling languages is often useful, e.g., to make tools (like simulators) based on one language applicable to models defined in other languages. However, several problems arise when the expressive powers of the modeling languages differ. We consider the automated transformation between models specified in the systems biology markup language (SBML) and ML-Rules, a rule-based multilevel modeling language. While both languages allow for modeling aspects that cannot be expressed in its counterpart and thus prevent a complete and fully automated transformation, it is still possible to transform many useful classes of models. Even more models can be transformed by relying on certain heuristics or user input.

MOTIVATION AND BACKGROUND

Automated model transformation from one formal language into another can be useful in many cases. For example, newly developed simulators need to be thoroughly tested regarding their correctness, for which many validated models might be required. However, independently validated test models are often encoded in a different language and translation into a suitable input format by hand can be tedious and error-prone. Another use case for model transformation is to reuse or extend a particular model in a way that can not be expressed in the language in which the original model has been described. In addition, the translation into another language might allow to use new analysis tools on the model. These benefits are multiplied if the transformation refers to a standardized and widely used model representation format.

Generally, a complete and sound translation from one format into another requires that the target formalism has the same or a greater expressive power than the source formalism, i.e., each aspect of the source language can be expressed with equal semantics in the target language. The challenge here is to identify which elements of the source language map on which target elements, and also to develop a general strategy for an according transformation. However, sometimes one might also want to transform a model from a certain language into a less expressive one, as typically not all language facilities are used in practice. Also, in some cases it might be permissible that certain aspects of the model can not be transformed correctly, e.g., if the transformed model shall be modified afterwards anyways. In such situations, it is important to know which aspects can be correctly transformed, where the limitations are, and what strategies are suitable if a completely correct transformation is impossible.

We investigate these issues in the context of a newly developed transformation mechanism between SBML (Hucka et al. 2003) and ML-RULES (Maus et al. 2011), a rule-based multilevel language available in the modeling & simulation framework JAMES II (Himmelspach and Uhrmacher 2007).

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RESULTS

A complete and correct transformation from SBML to ML-RULES can be achieved in many cases. For example, our approach allows to successfully transform 249 of 432 curated models from the BioModels database (Le Novère et al. 2006); version of July 9th, 2012. Problems arise if some special language features are used in SBML models that have no syntactical and semantical counterparts in ML-RULES, e.g., referencing the simulation time within a model. Although ML-RULES is generally more expressive than SBML and thus many SBML models can be successfully transformed, the according process is not a trivial task. As ML-RULES allows to express hierarchical relationships between model entities, this has to be accounted for in the transformation of SBML reactions. Moreover, all variables used in mathematical expressions need to be provided by a rule's reactants, which may require to add additional reactants (and products).

On the other hand, converting a model from ML-RULES to SBML poses even greater challenges, as ML-RULES species may have an arbitrary number of attributes, they may build up a hierarchy of arbitrarily nested species, and rules may rely on complex patterns including flexible constraints. Therefore, ML-RULES models may implicitly define countably infinite sets of species and reactions. This prevents an exact transformation to SBML models, as these need to explicitly specify each possible combination of attributes as well as hierarchical locations (and all reactions on them). Such problems can only be solved heuristically — e.g., we rely on a directed graph to search possible attribute combinations for an ML-RULES species that could be generated with the existing rules. The heuristics can be configured by the user.

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