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Managing Computational Models and Associated Simulation Descriptions in Standard Formats

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Motivation

The number of publicly available simulation models increases rapidly. Model reuse and simulation result reproduction have therefore become important tools for the systems biology community [1]. Different model repositories provide access to model code and model meta-information. However, the application of database and information systems techniques can enhance the work with such repositories and thereby improve the reuse of available models [2]. We argue that the integration of model-related information will further support the process of modeling in systems biology.

Model: A computational model of a biological system, annotated with meta-information and stored in XML format [2]

Meta-Information: Additional (third-party) knowledge about the modeled system (encoded as annotations), e.g. model author, modification dates, or model entity descriptions in ontologies

Storage

Version Control

Models evolve over time. Providing the complete history of a model enables users to understand the model's development steps and to follow on model updates [3].

Requirements:

• Track changes in models

- Access to all model versions
- Explanation of changes

Solutions:

- Model diff: BiVeS
- Visualization and model evolution: BudHat

Ranked Retrieval

We promote to apply Information Retrieval techniques to retrieve relevant models from the graph store. The proposed ranking and retrieval techniques focus on the processing of model meta-information [2].

Requirements:

• Search results be ranked by relevance • Similarity by determining model features • Integration of different types of model related data

Solutions:

 Vector Space Model • Weight concept to satisfy different user requirements

Availability

All approaches are format independent and can therefore be applied to models in different model representation formats. We develop open code and make all our tools available for testing. http://sems.uni-rostock.de/

References

[1] Waltemath et al. (2011) BMC Systems Biology, 5:198 [3] Waltemath et al. (2013) Oxford Bioinformatics [4] Henkel et al. (2012) INFORMATIK2012 [2] Henkel et al. (2010) BMC Bioinformatics **11**:423

