

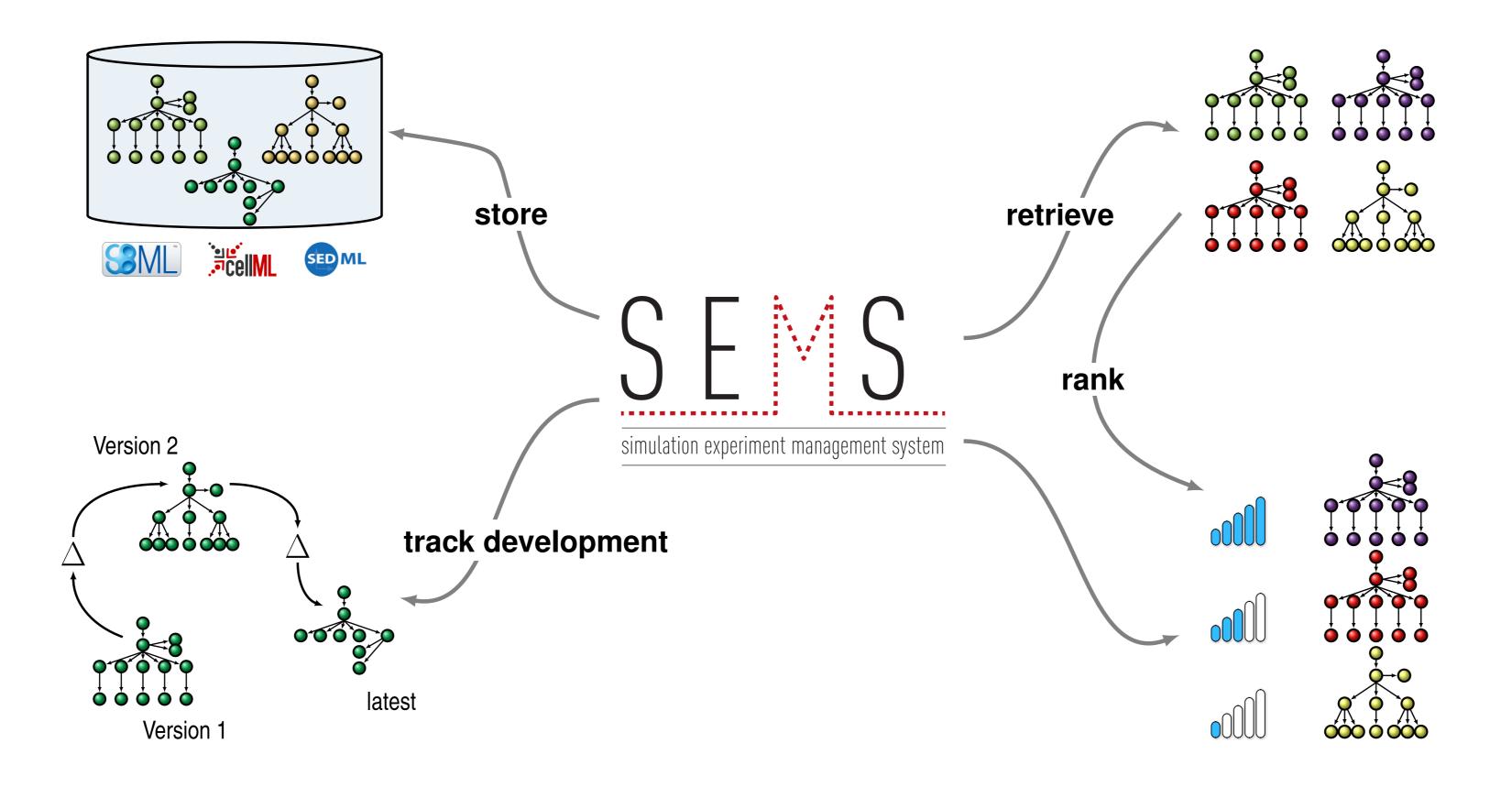


## The SEMS Project: Managing Simulation Models

Overview

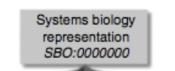
SEMS is a BMBF-funded e: Bio project dedicated to the development of methods and tools for improved management of computational models and associated simulation setups in standard

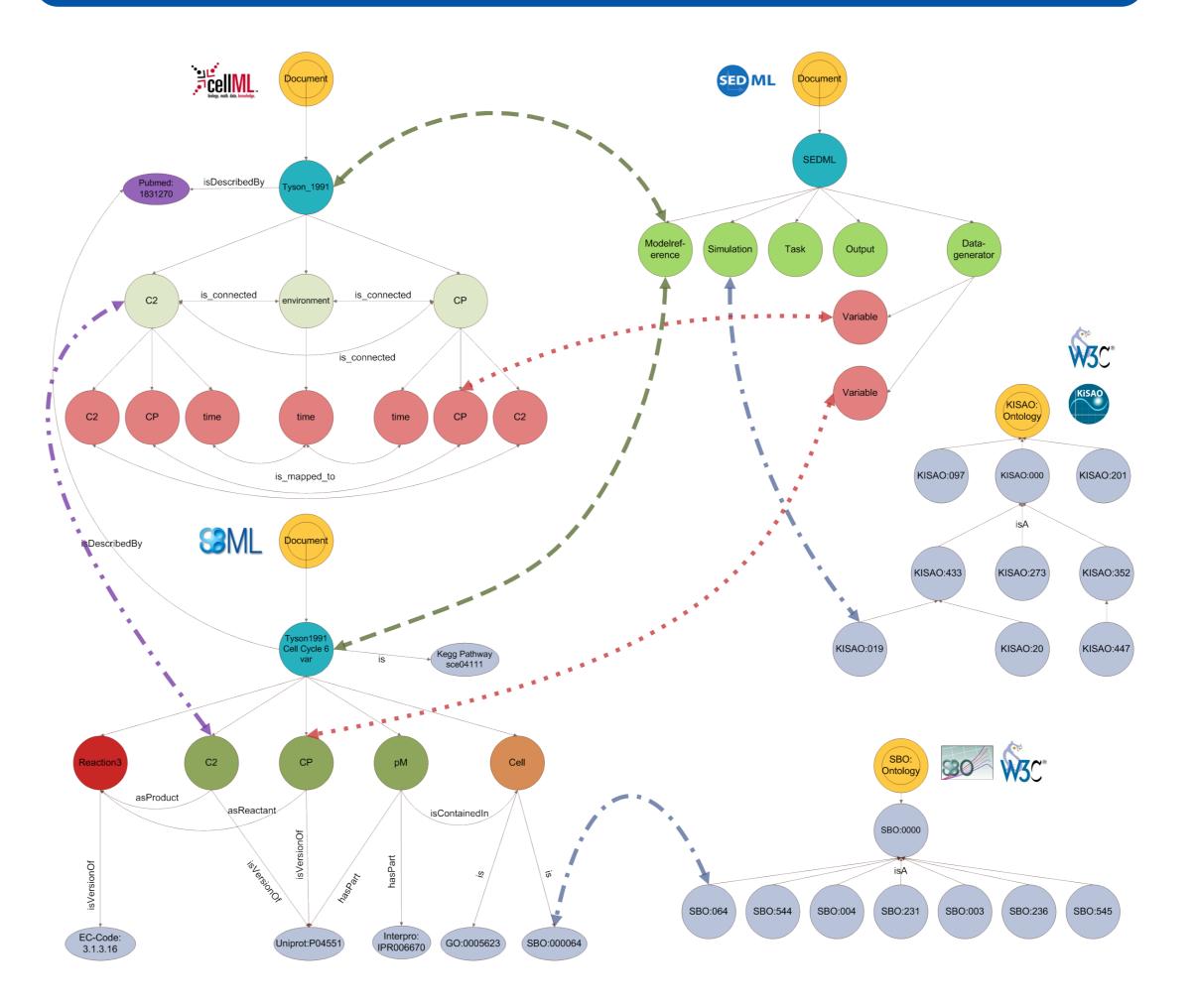
formats. The SEMS-team is a group of young researchers who care for model storage and retrieval (Ron Henkel), model version control (Martin Scharm), the encoding of models and simulation setups (Martin Wolfien), and the development of software applications (Martin Peters).

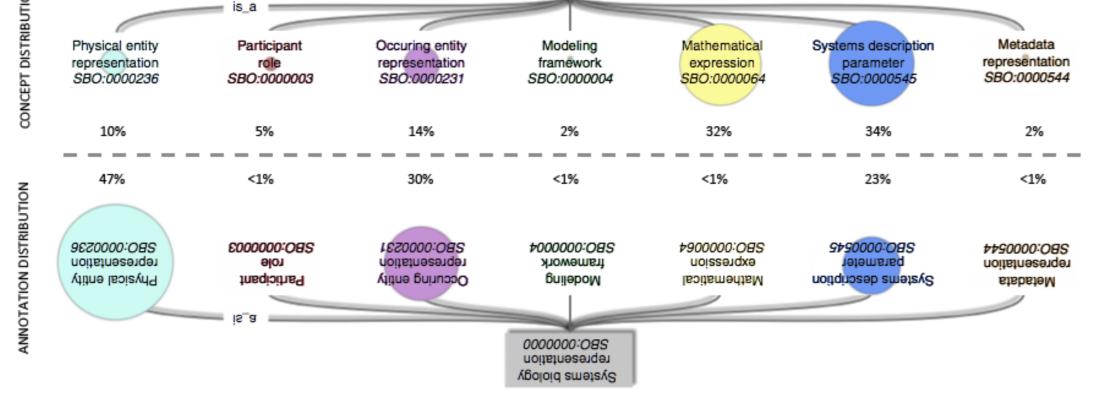


## Feature extraction from model annotations

## Linking models and simulation descriptions

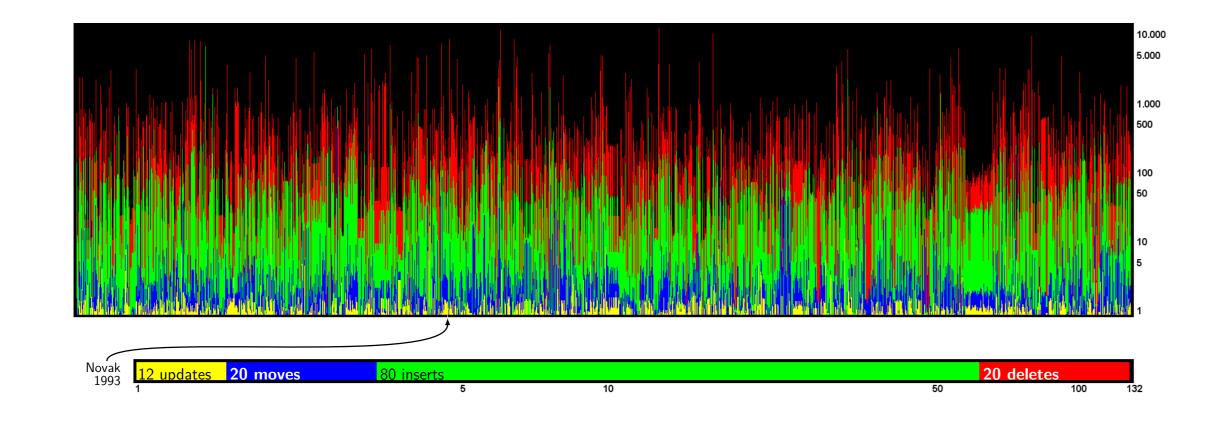






**Overview of concept distribution in SBO.** The figure shows the distribution of concepts in the seven branches of the Systems Biology Ontology (SBO, Figure adapted from [2]). The size of the colored circles visualizes the number of concepts summarized by each branch. The bottom mirrored image visualizes the distribution of annotations from all models in the BioModels Database. (Figure originally published in [1])

## Changes in model versions



**Sketch of links between different types of documents** as represented in our graph database (Neo4j): simulation experiment descriptions and models (dashed line); defined observation variables and model entities (dotted line); annotated model entities and simulation experiment descriptions (dashed-dotted line); and model entities of different representation formats (double dotted-dashed line). (Figure taken from [3])

**Statistics on model updates in the CelIML Model Repository.** The figure shows the updates in all versions of all models currently published in the CelIML Model Repository. Each bar on the x-axis corresponds to a diff between two consecutive versions of the same model. Y-axis shows the total number of identified changes (yellow: update; blue: move; green: insert; red: delete). Data generated with BiVeS [4], Figure courtesy Martin Scharm.

[1] Rebekka Alm et al. Annotation-based feature extraction from sets of sbml models. In *Databases in the life sciences (DILS), accepted for publication*, 2014.
[2] Mélanie Courtot et al. Controlled vocabularies and semantics in systems biology. *Molec-*

ular systems biology, 7(1), 2011.

- [3] Ron Henkel et al. Combining computational models, semantic annotations, and associated simulation experiments in a graph database. *in preparation*, 2014.
- [4] Dagmar Waltemath et al. Improving the reuse of computational models through version control. *Bioinformatics*, 29(6):742–748, 2013.



Ron Henkel ron.henkel@uni-rostock.de



Martin Scharm martin.scharm@uni-rostock.de



Dagmar Waltemath dagmar.waltemath@uni-rostock.de



Olaf Wolkenhauer@uni-rostock.de

