# CombineArchive Toolkit

Sharing in silico experiments is essential for the advance of research in computational biology. The COMBINE archive is a digital container format to easen the management of numerous files and to enable the exchange of reproducible modelling results. We developed the CombineArchive Toolkit, consisting of a library, a web interface and a desktop application. It support scientists in creating, exploring, modifying, and sharing COMBINE archives.
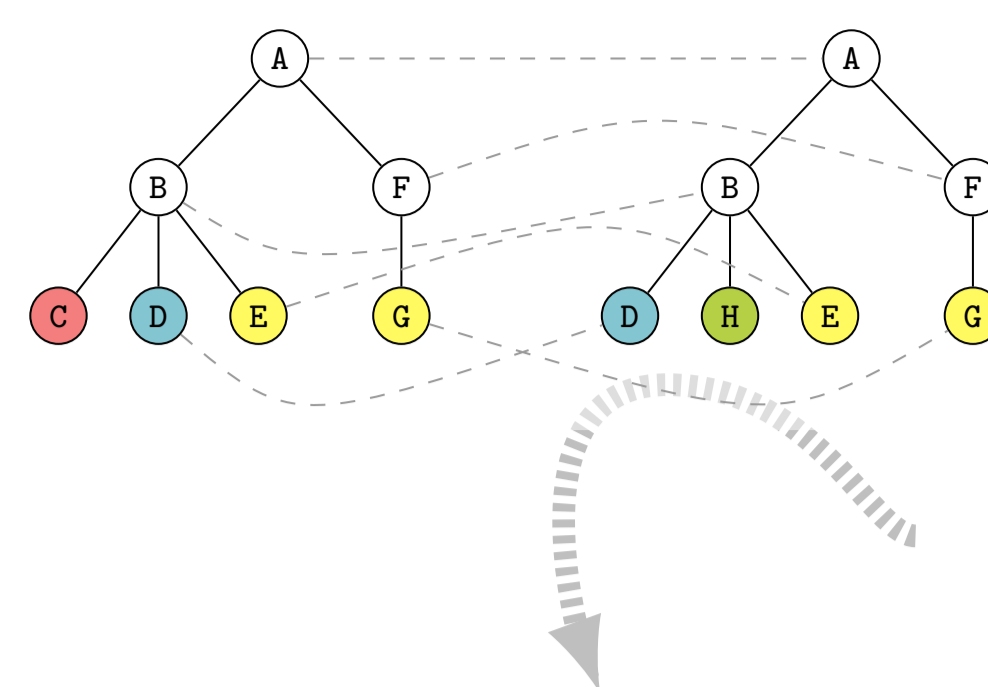
BiVeS

Armed with our method for difference detection, BiVeS is able to detect and communicate the differences in computational models. The differences are exported in several machine- and human-readable formats, ideally suited to be integrated in other tools.

BudHat

BudHat showcases how BiVeS improves the understanding of a model's changes. BudHat calls BiVeS for the comparison two versions of a computational model and displays the obtained results in the web browser.
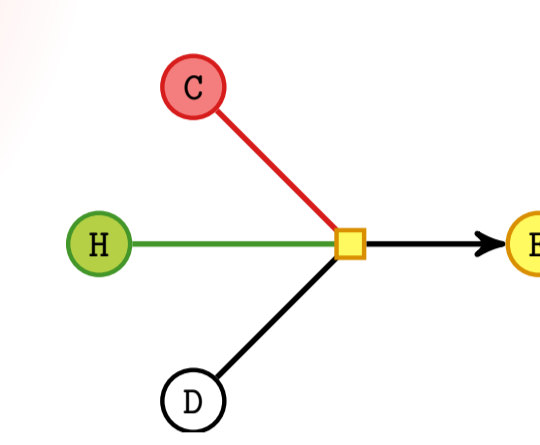
Version Control for Computational Models

With thousands of models available, a framework to track the differences between models and their versions is essential to compare and combine models. Focusing on SBML and CellML, we developed an algorithm to accurately detect and describe differences between versions of a model with respect to (i) the models' encoding, (ii) the structure of biological networks, and (iii) mathematical expressions.

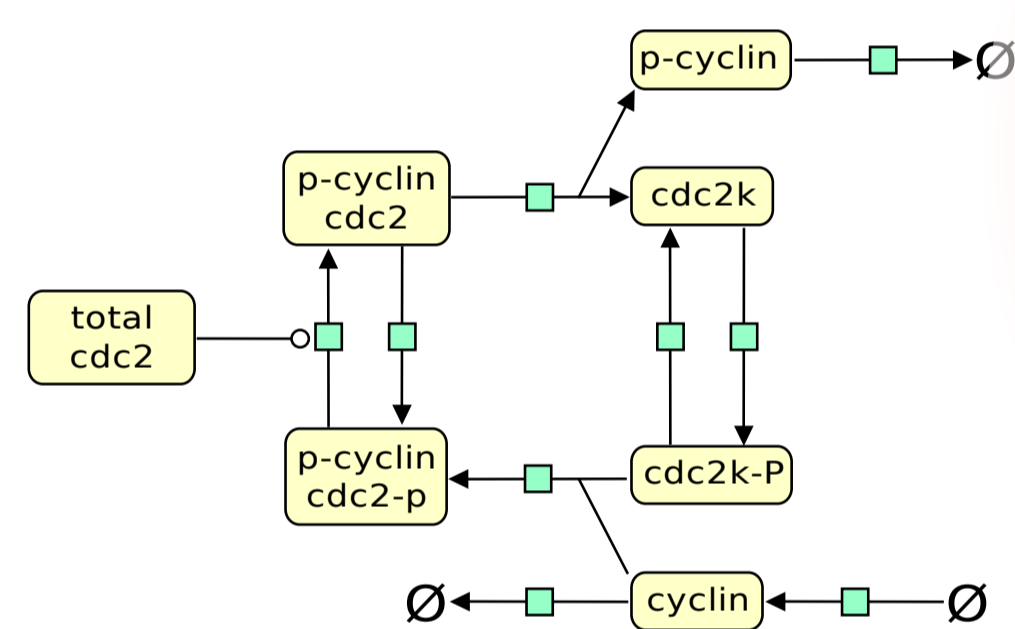version x-1   version x   version x+1
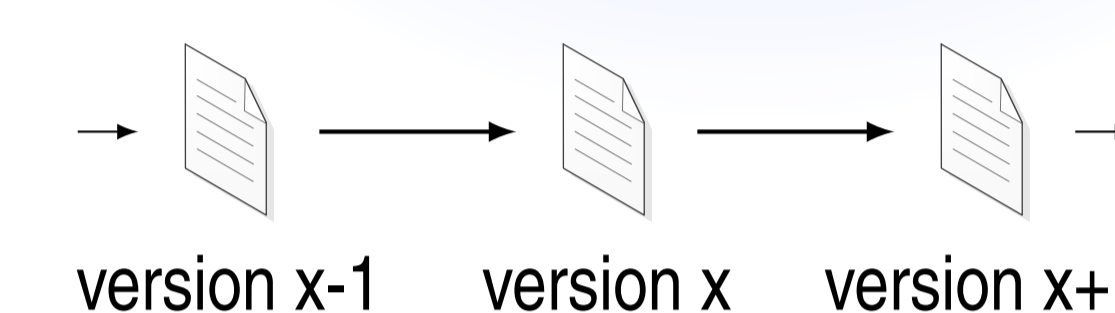
de.NBI Infrastructure

We will provide data management and support for systems biology projects, with a focus on provenance and reproducibility of experimental and modelling results. *de.NBI:SYSBIO* is part of a large German Network for Bioinformatics Infrastructure. **WE ARE HIRING!**

SBGN-ED

SBGN is a markup language to describe models and exchange information about biological systems graphically. We will further develop methods and tools for SBGN-compliant visualisation of model-related information. **WE ARE HIRING!**
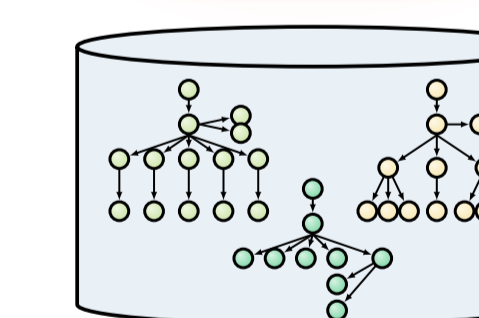
Ontology of Differences

Changes in model versions are manifold and appear on different layers. We develop an ontology of differences occurring in model versions. It will support researchers in analysing differences, discovering typical changes, summarising major changes and providing statistics.

2MT

2MT is our web based platform to demonstrate the capabilities of SEMS-related tools. It exemplifies how our model management solutions can be used in existing tools.

S E M S
simulation experiment management system
https://sems.uni-rostock.de

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Masymos

Containing SBML- and CellML models, linked semantic annotations (e.g., from bio-ontologies), simulation descriptions, graphical representations and other available types of model-related data, out graph database Masymos can now be queried for complete simulation experiments.

Models as graphs

The increasing diversity of model-related data that is necessary to perform a simulation study leads to new challenges in model storage. We developed a concept for graph-based storage of models and model-related data. Graphs reflect the models' structure much better, enable linking of model-related data on the storage layer, and allow for an efficient search.

Morre

Our retrieval engine for models applies Information Retrieval techniques to retrieve relevant models from MASYMOS. The proposed ranking and retrieval techniques focus on the processing of model meta-information.

Improving the Management of Simulation Studies in Computational Biology
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