Towards model version control

Dagmar Waltemath

SEMS

simulation experiment management system

SYSTEMS BIOLOGY BIOINFORMATICS ROSTOCK

Universität Rostock

Traditio et Innovatio

gegründet 1419

Versions of models

Evolution of a model over time

Waltemath et al. (submitted)

Information in BioModels Database

version 1   current version

Directly accessible from the repository:

– Original model file (any format)

– Current model file

– Date of creation and last modification

version 1   current version

release 1   release 2

Implicitly accessible:

– Model file(s) at each BioModels Database release

Information in PMR2

You are here: Home > Exposures > Novak, Tyson, 1993 > Numerical analysis of a comprehensive model of M-phase control in Xenopus oocyte extracts and intact embryos: parameter values have been taken from the original published paper to reproduce figure 4A.

Numerical analysis of a comprehensive model of M-phase control in Xenopus oocyte extracts and intact embryos: parameter values have been taken from the original published paper to reproduce figure 4A.
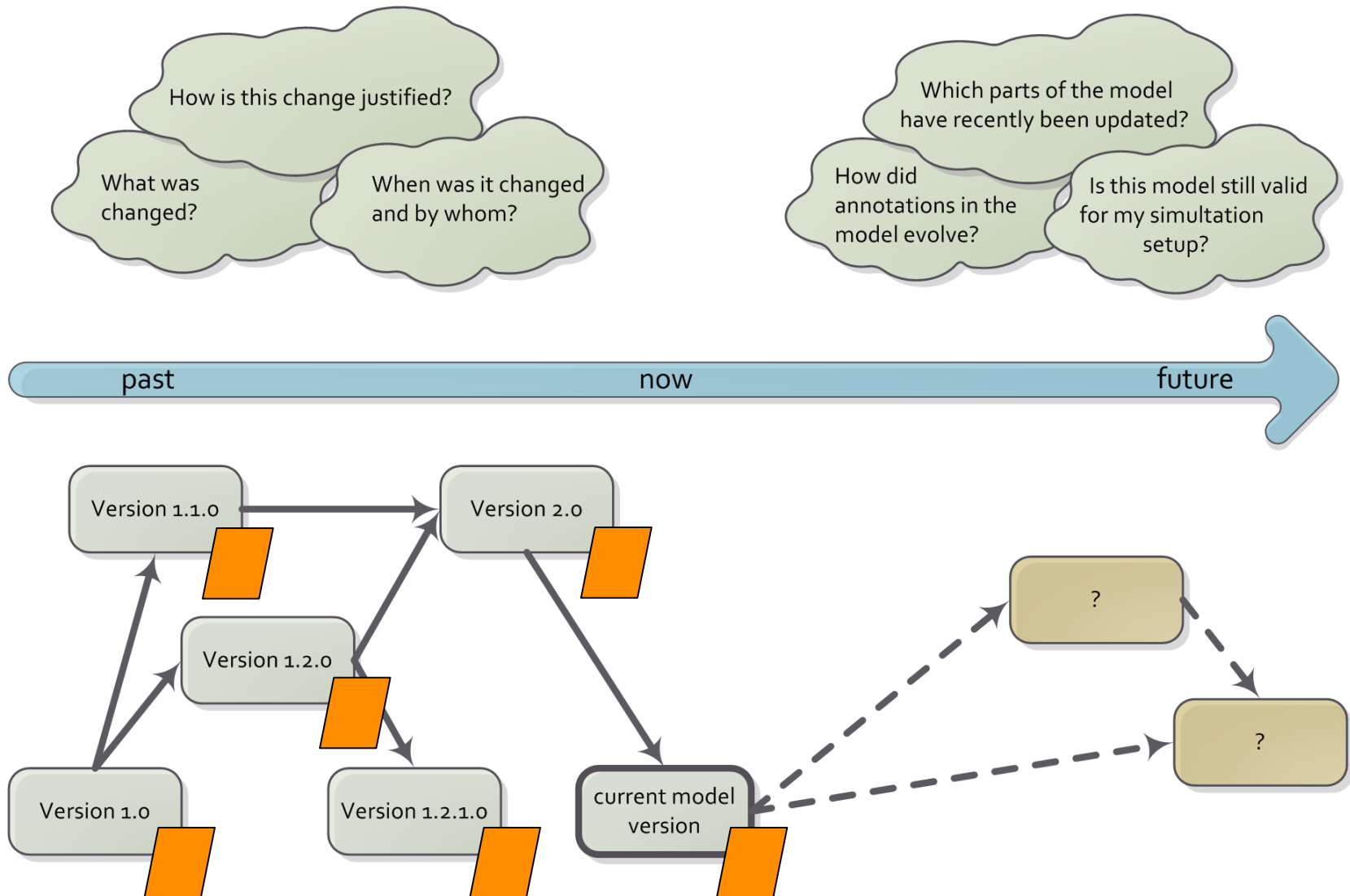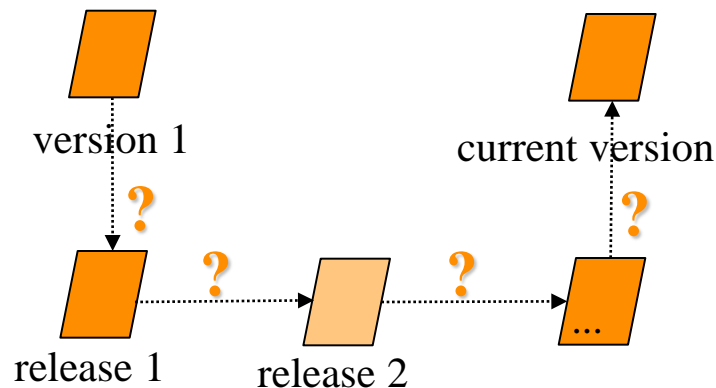
Model Status

This CellML version of the model has been checked in COR and OpenCell. This variant of the model runs to replicate the original published results as depicted in figure 4A of the paper. Please note that actual concentrations are displayed by this model, instead of the percentage concentrations used in the paper. The units have been checked and they are consistent.

Model Structure

ABSTRACT: To contribute to a deeper understanding of M-phase control in eukaryotic cells, we have constructed a model

Model Curation

Curation Status:
OpenCell:
JSim:
COR:

Source

Derived from workspace Novak, Tyson, 1993 at changeset a39b4d26855a.
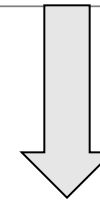
You are here: Home > Workspaces > Novak, Tyson, 1993

Log in | Register

| view | log | shortlog | manifest |

Changelog Entries

- (0)
- tip

Date	Author	Log
2010-07-05 22:14 +1200		Updated documentation and added meaningful names to the two model variants.
2010-07-05 14:24 +1200		Tidied session file
2009-11-25 14:00 +1300		Added images in ai svg and png format
2009-11-10 10:39 +1300		Removed non pub med reference
2009-11-10 09:32 +1300		Added keyword
2009-06-17 15:26 +1200		committing version02 of novak_tyson_1993
2009-01-14 04:19 +1300		committing version01 of novak_tyson_1993

cellML
biology. math. data. knowledge.

– CellML metadata specification

   – http://www.cellml.org/specifications/metadata/

   – Elements from rdf, dc, dcterms, vcard

   – Trivial vs substantial changes

– SBML History concept

   – dc:creator *model creators*

   – dcterms:created *creation date*

   – dcterms:modified *modification date*

Version information is not propagated to the users.

Currently used algorithms are not suitable for difference detection in XML models (SBML, CellML, NeuroML).

- Find the difference between two model versions,

- understand what a change is about,

- and understand why a model update had been necessary.

1. XML-aware algorithm for difference detection
2. Transparent changes
3. Justification for changes

```
 1 @@ -661,13 +661,11 @@
 2 [...]
 3 -        <rdf:Description rdf:about="#_905882">
 4 -          <bqbiol:isVersionOf>
 5 -            <rdf:Bag>
 6 -              <rdf:li rdf:resource="urn:miriam:obo.go:GO%3A0043037"/>
 7 -            </rdf:Bag>
 8 -          </bqbiol:isVersionOf>
 9 -        </rdf:Description>
10 +<rdf:Description rdf:about="#_905882">
11 +<bqbiol:isVersionOf><rdf:Bag>
12 +<rdf:li rdf:resource="urn:miriam:obo.go:GO%3A0043037"/>
13 +</rdf:Bag></bqbiol:isVersionOf>
14 +</rdf:Description>
15 [...]
```

**SYSTEMS BIOLOGY
BIOINFORMATICS
ROSTOCK**

- Detects all diffs
    - insert, delete, update, move
    - for two model files,
    - typically two versions of the same model
- Adaptation of *XyDiff*,
    - entity-based
    - ignores XML formatting
    - http://leo.saclay.inria.fr/software/XyDiff/

```
Diff:
  <updates>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='Cdc25_Reaction']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='Cdc2Phos']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='G1R_Binding']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='G2R_Creation']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='IE_Reaction']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='PG2R_Creation']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='UbE2_Reaction']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='UbE_Reaction']" elementName="reaction"/>
    <attribute attributeName="reversible" value="true" oldValue="false"
        path="[@id='Wee1_Reaction']" elementName="reaction"/>
  </updates>
```

Waltemath et al. (submitted)

2. Transparent changes: model history

Table 1: Version information about model BIOM007

Revision	Date	SVN Comment
R2* initial	06/16/2009	original models.
R3*	06/16/2009	the latest version when implementing revision control
R37	07/29/2009	four assignment rules (k2, k6, kwee and k25) were changed to function definitions.
R51	08/10/2009	converted to SBML Level2 Version 4 and curated. Attributes 'spatialSizeUnits' in element, and 'timeUnits' and 'substanceUnits' in element, which are not part of SBML Level 2 Version 4 element are eliminated.
R57	08/13/2009	The model should remain in SBML L2V1. The model was integrated and simulated using Mathematica 6.0 - MathSBML 2.7.1, which does not support SBML L2V4.
R194	10/15/2009	corrected one error in a kinetic law (Ube1 activation) and changed the file a bit to get it to l2v3 [line break] recurated it, but still problems with the initial conditions

Waltemath et al. (submitted)

Model history (version tree)

– Diff list

– *adapted from Rosado et a., 2009 (EDBT)*
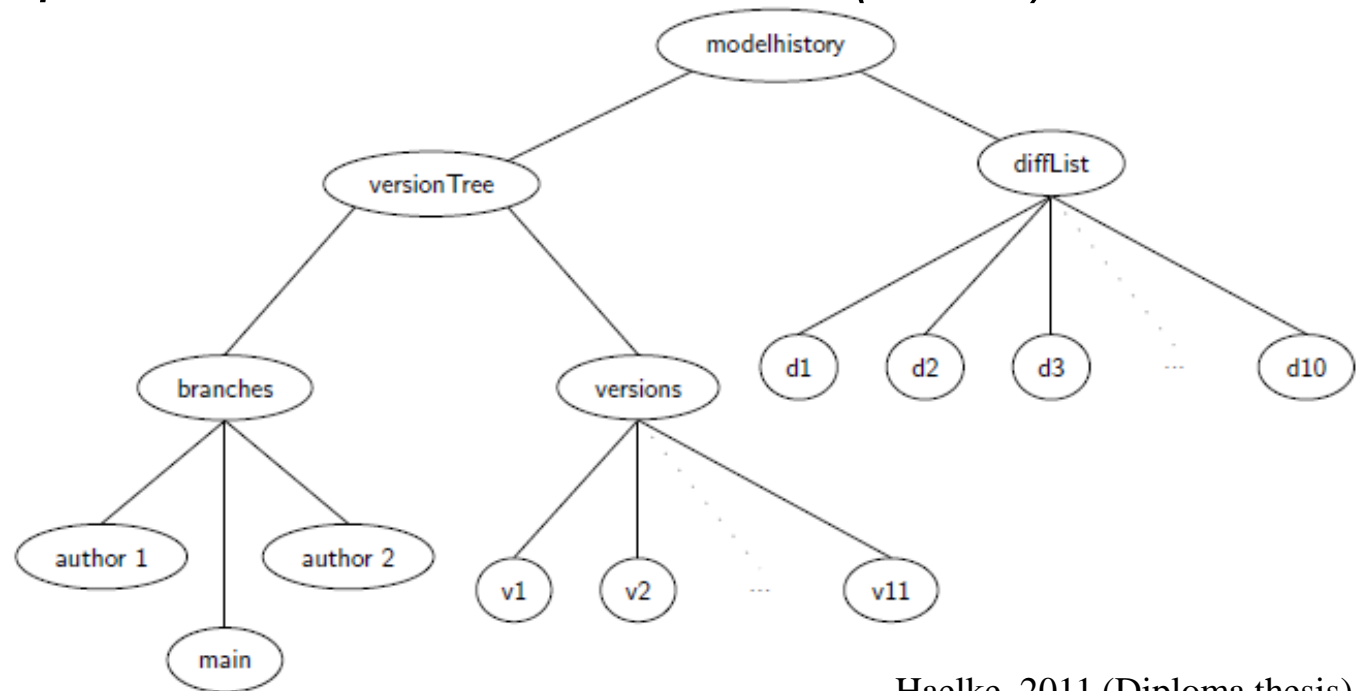
Haelke, 2011 (Diploma thesis)

**SYSTEMS BIOLOGY
BIOINFORMATICS
ROSTOCK**

Controlled vocabulary for annotation of the diff file
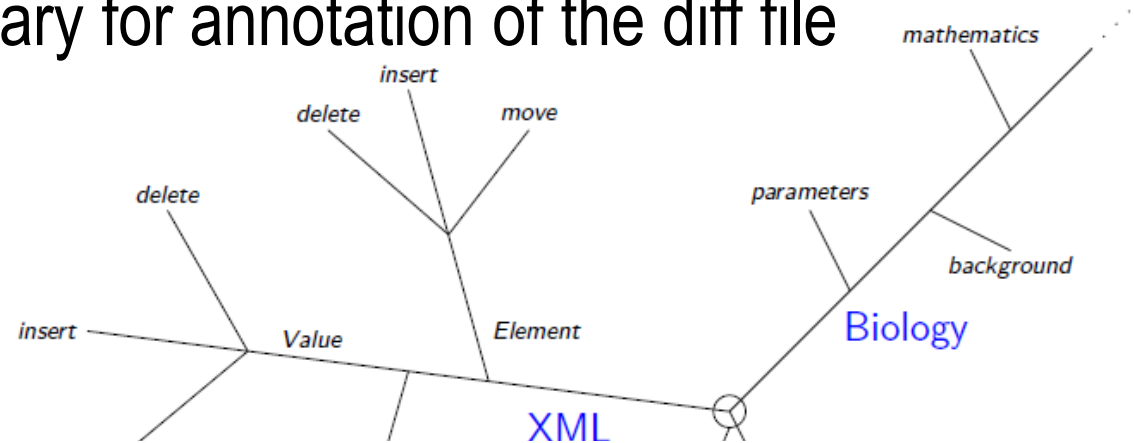
Table 2: Controlled vocabulary for types of changes.

Location		Type	Operation
XML element attribute value	Annotation qualifier URI	mathematics biology parameter typo . . .	update insert delete move

Haelke, 2011 (Diploma thesis)

Waltemath et al. (submitted)

Biochemical Model Versioning System (BiVeS)

Waltemath et al. (submitted)

- Java library for diffList and model history

- Can be used on top of SVN/Mercurial systems to store differences between two model versions, and maintain a history of versions

- Tested on: SBML@BioModels Database

- https://bitbucket.org/rhaelke/bives.fwk/overview

BudHat: a web-based diff tool

- – Tree-based view of model versions (history)

- – Difference between two models

- – XML representation (diff format)

- – Graphical representation (GraphViz)

http://www.sbi.uni-rostock.de/budhat
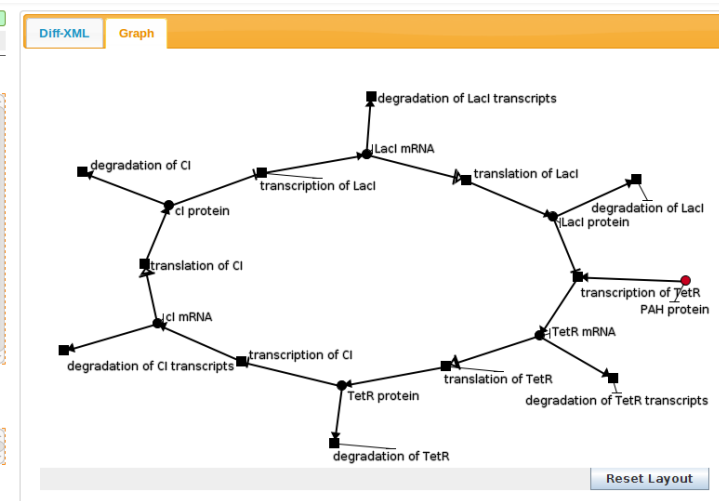
- Targeting single versions of a model (model version IDs), e.g. to build the model history

- Change annotation

- Detecting merges in models

- Support of CellML, NeuroML, SED-ML etc in the diff tool

Systems Biology and Bioinformatics, Rostock