

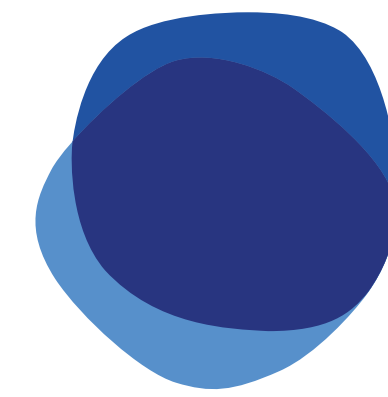
dcterms:title="COMputational MOdels DIffer"

dcterms:description="hands-on-poster"

Universität
Rostock



Traditio et Innovatio



SYSTEMS BIOLOGY
BIOINFORMATICS
ROSTOCK

SEMS
simulation experiment management system

take a pen and jot down
whatever comes to your mind!

prov:generalizationOf

Change

Insertion of:

```
<species name="Gulcose" initialConc="0.6" />
```

BiVeS detects

```
<insert>
  <node id="13" newTag="species" [...] />
  <attribute id="14" triggeredBy="1"
    name="initialConc" newValue="0.6" [...] />
  [...]
</insert>
```

Annotation using COMODI

```
#13 a comodi:Change;
    comodi:hasChangeType comodi:Insertion;
    comodi:affects comodi:ReactionNetworkDefinition;
    comodi:hasIntention comodi:Expansion.
#14 a comodi:Change;
    comodi:hasChangeType comodi:Insertion;
    comodi:hasIntention comodi:Expansion;
    comodi:affects comodi:SpeciesSetup;
    comodi:wasTriggeredBy #13.
```

Update of:

```
<species name="Gulcose" initialConc="0.6" />
<species name="Glucose" initialConc="0.6" />
```

```
<update>
  <attribute id="23" newValue="Glucose"
    name="name" oldValue="Gulcose" />
  [...]
</update>
```

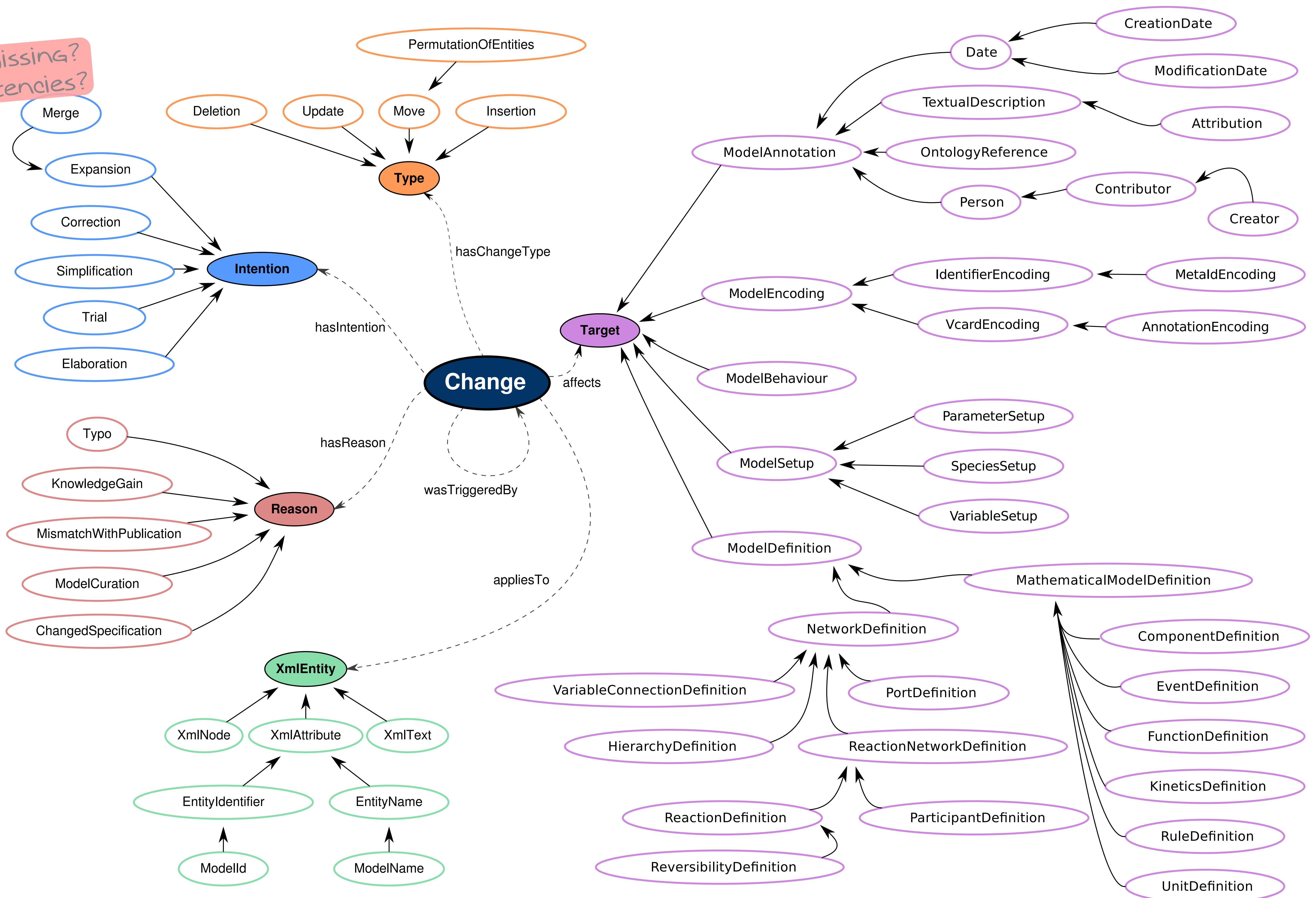
Update of:

```
<parameter name="ka" value="0.3" />
<parameter name="ka" value="0.1" />
```

```
<update>
  <attribute id="42" name="value" newValue="0.1" oldValue="0.3" />
</update>
```

```
#42 a comodi:Change;
    comodi:hasChangeType comodi:Update;
    comodi:appliesTo comodi:XmlAttribute;
    comodi:affects comodi:MathematicalModelDefinition;
    comodi:hasIntention comodi:Correction;
    comodi:hasReason comodi:MismatchWithPublication.
```

terms missing?
inconsistencies?



dcterms:abstract

Models are regularly updated, even after publication. The BiVeS library [3, 4, 5] offers comparison of versions of SBML [6] and CellML [7] encoded models. The result of such a comparison is a list of changes, based on the differences in both XML files. While it is now easy to see the differences in a network, it is still not possible to provide - or retrieve - information about the causes and effects of these changes. For example, together with a model update it should be possible to provide information on the characteristics of a change, e.g. stating that the changes remove an error in the kinetics.

We manually analysed hundreds of model versions and their differences from the BioModels Database [9] and the CellML Model Repository [8] to study the evolution of computational models. We then derived a vocabulary to describe the differences and implemented it in the COMODI ontology. The OWL encoding and a documentation are available from our website [1]. A Java library [2] allows for easy integration in software projects. We envision to use COMODI for automatic annotation of differences generated in BiVeS, and we like to provide it to modellers who wish to document the evolution of their models.

pdfs: seeAlso

- [1] <http://purl.org/net/comodi>
- [2] <https://github.com/bioinformatics/comodi>
- [3] <https://sems.uni-rostock.de/bives/>
- [4] Scham et al.: An algorithm to detect and communicate the differences in computational models describing biological systems Bioinformatics, 2015.
- [5] Waltemath et al.: Improving the reuse of computational models through version control Bioinformatics, 2013.
- [6] Hucka et al.: The Systems Biology Markup Language (SBML): A medium for representation and exchange of biochemical network models Bioinformatics, 2003.
- [7] Lloyd et al.: CellML: its future, present and past Progress in Biophysics and Molecular Biology, 2004.
- [8] Lloyd et al.: The CellML Model Repository Bioinformatics, 2008.
- [9] Li et al.: BioModels Database: An enhanced, curated and annotated resource for published quantitative kinetic models BMC Systems Biology, 2010.

up for a discussion? contribution?
collaboration? or just a beer?
if i'm not currently at the poster
just drop me a line and i'll come over



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