dcterms:title=“**CO**mputational **MO**dels **DI**ffer“

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" />
```

Update of:

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

Update of:

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

BiVeS detects

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

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

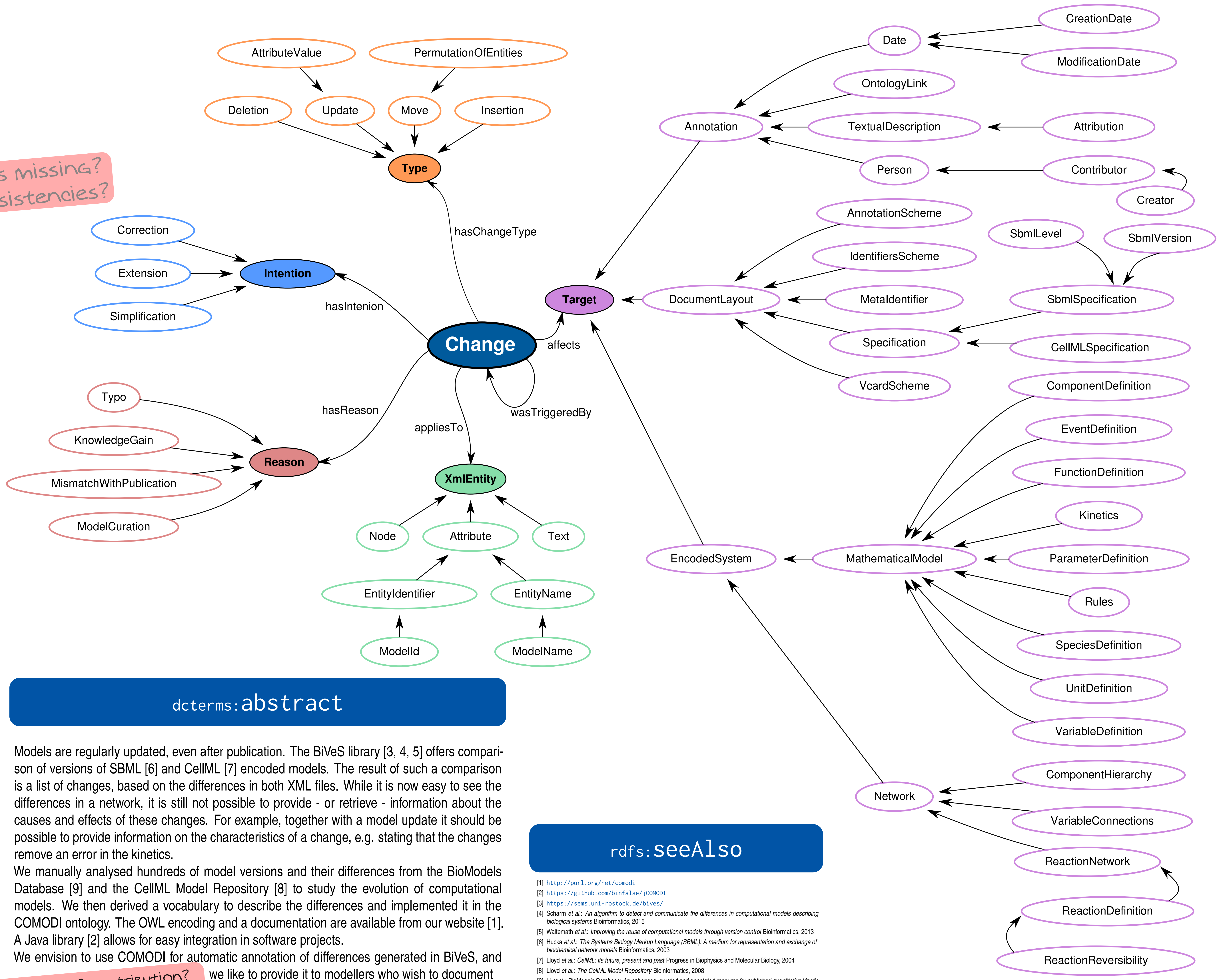
```
<update>
  <attribute id="42" name="value" newValue="0.1" oldValue="0.3" />
</update>
```

Annotation using COMODI

```
#13 a comodi:Change;
    comodi:hasChangeType comodi:Insertion;
    comodi:affects comodi:ReactionNetwork;
    comodi:hasIntention comodi:Extension.
#14 a comodi:Change;
    comodi:hasChangeType comodi:Insertion;
    comodi:hasIntention comodi:Extension;
    comodi:affects comodi:Kinetics;
    comodi:wasTriggeredBy #13.
```

```
#23 a comodi:Change;
    comodi:hasChangeType comodi:Update;
    comodi:appliesTo comodi:EntityName;
    comodi:hasReason comodi:Typo.
```

```
#42 a comodi:Change;
    comodi:hasChangeType comodi:Update;
    comodi:appliesTo comodi:Attribute;
    comodi:affects comodi:MathematicalModel;
    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 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.

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

rdfs:seeAlso

[1] http://purl.org/net/comodi
[2] https://github.com/binfalse/jCOMODI
[3] https://sems.uni-rostock.de/bives/
[4] Scharm *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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