Universität Rostock Traditio et Innovatio

SYSTEMS BIOLOGY BIOINFORMATICS ROSTOCK

SEMS simulation experiment management system

Standardized visualization of differences between model versions

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Department of Systems Biology and Bioinformatics, University of Rostock

the combine computational modeling in biology network

COMBINE 2016
Newcastle upon Tyne
23rd of September 2016

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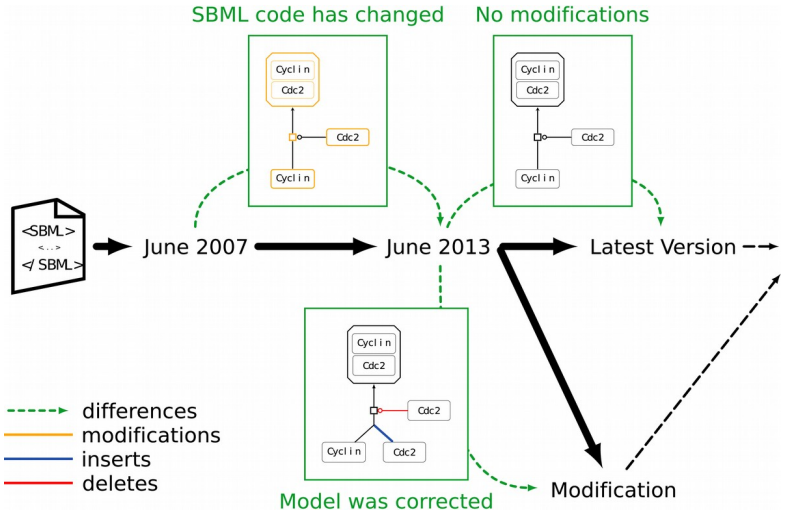
Motivation: models are evolving

Biological models are constantly evolving implying that several versions of a model can exist.



Scharm et al. (2015) An algorithm to detect and communicate the differences in computational models describing biological systems - *Bioinformatics*.

Figure courtesy: Tom Gebhart

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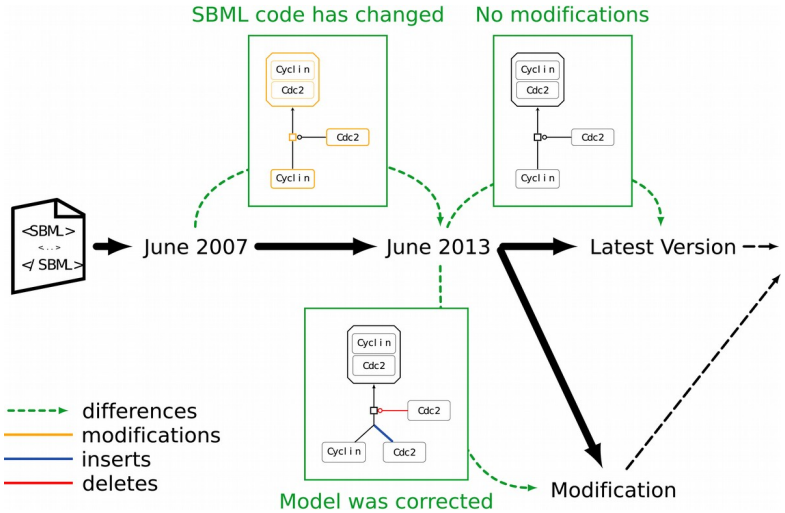


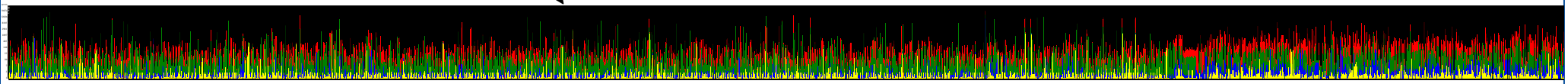
Scharm et al. (2015) An algorithm to detect and communicate the differences in computational models describing biological systems - *Bioinformatics*.

Statistics based on two repositories of computational models: Physiome and Biomodels.

Number of models: 3237

Number of model versions: 14439

Number of deltas: 10662

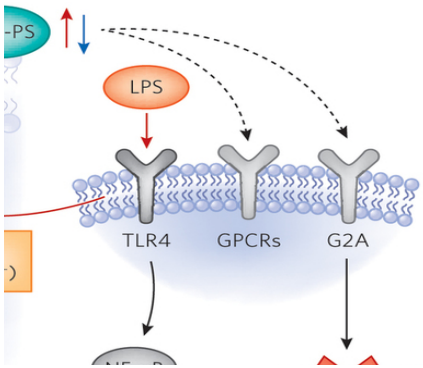


http://most.sems.uni-rostock.de/

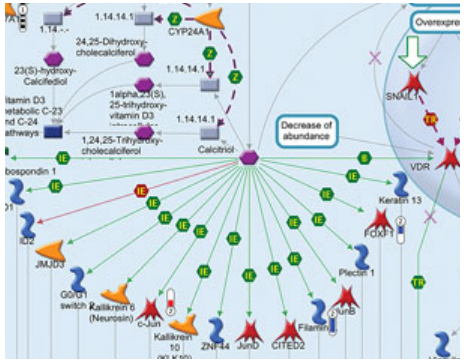
Figure courtesy: Tom Gebhart

Motivation: visualizing models

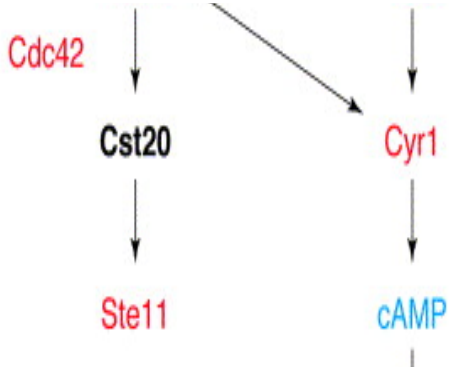
Plus, it is common to have a visual representation of biological networks…



H. Kim (2015), Nature Chemical Biology



Systems Biology Tools for Integrated Omics Analysis - M. Hugues



Brown et al. (1999), Trends in Microbiology

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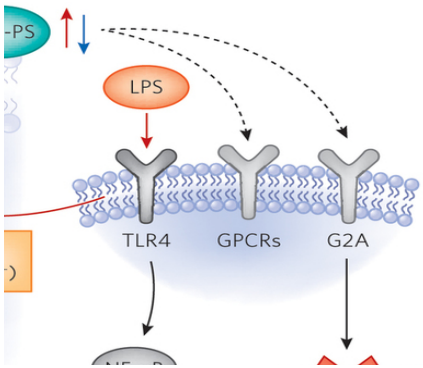

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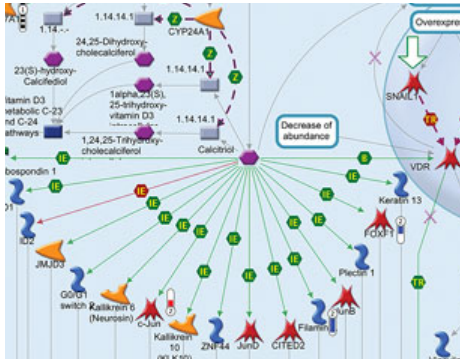

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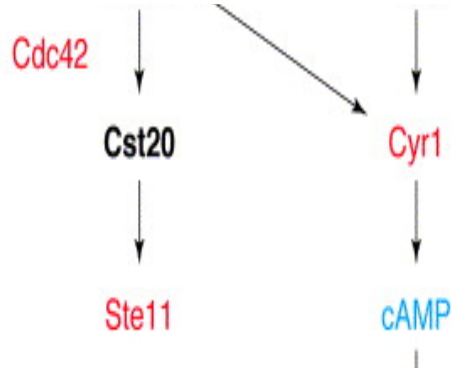
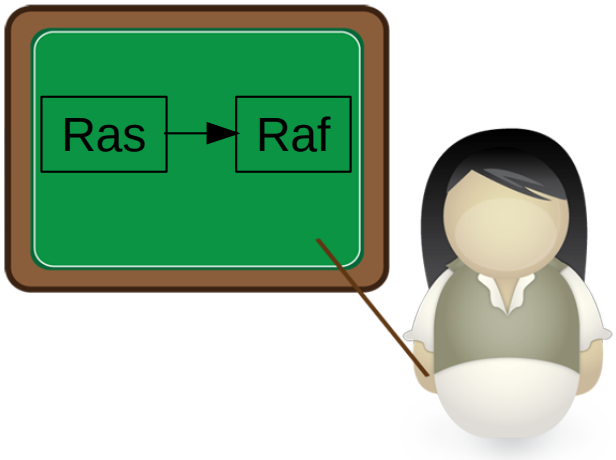


Brown et al. (1999), Trends in Microbiology

… but understanding them depends on the reader's knowledge …



Ras translocates Raf

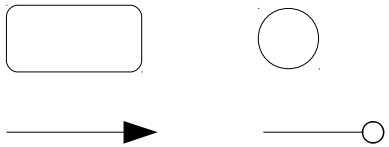
Ras activates Raf

Ras recruits Raf

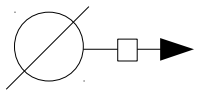
The Systems Biology Graphical Notation

… unless the Systems Biology Graphical Notation is used.

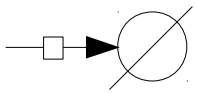
standardized glyphs and arcs



and semantics specific to each.



source



sink

The Systems Biology Graphical Notation

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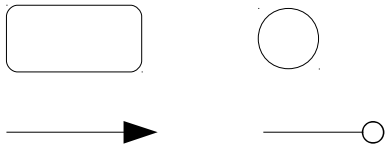

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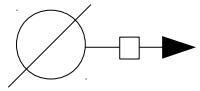
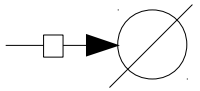
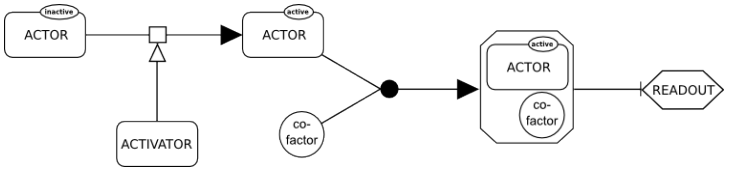




Three languages are defined.

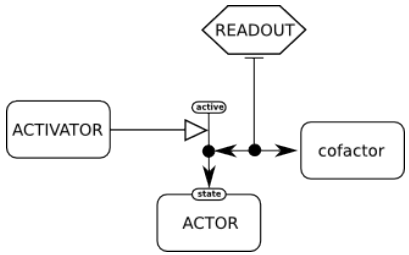
Process Description

Biochemistry



Entity Relationship

Physiology, Genetics



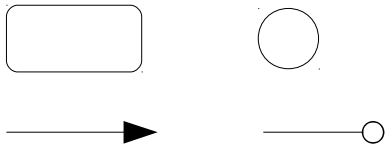
Activity Flow

Molecular biology

The Systems Biology Graphical Notation

… unless the Systems Biology Graphical Notation is used.

standardized glyphs and arcs



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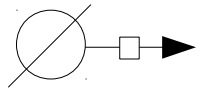

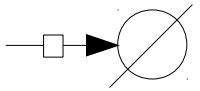

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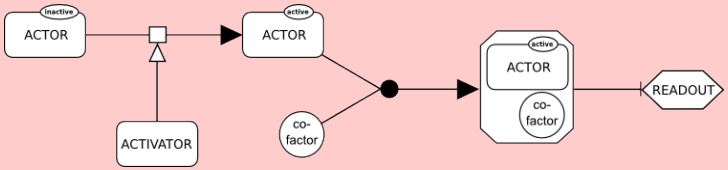

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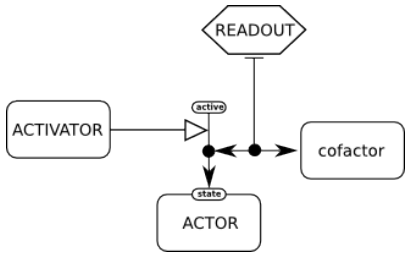

Activity Flow

Molecular biology

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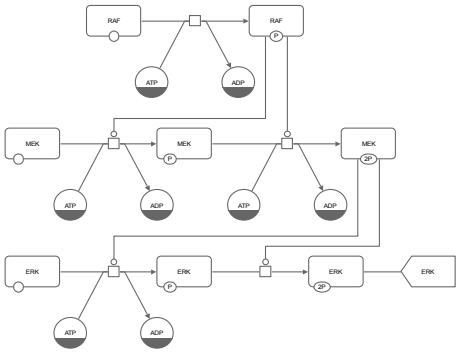
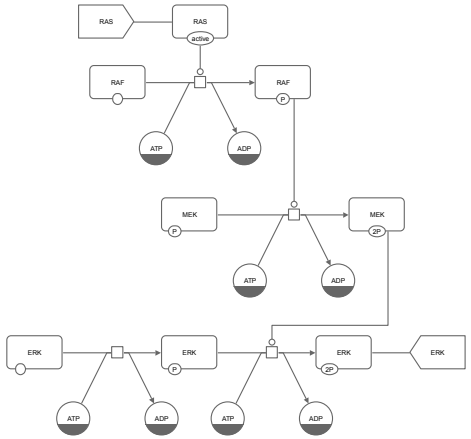
Objective: standardize diffs visualization

Highlighting of the differences between two model versions using SBGN.



Version 1



Version 2

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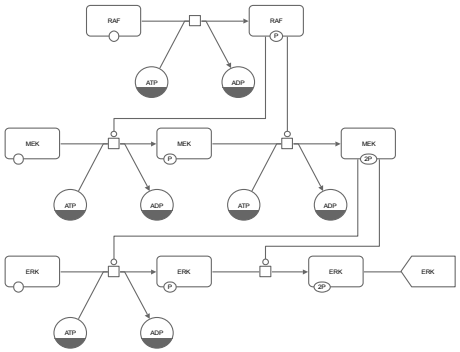
Objective: standardize diffs visualization

Highlighting of the differences between two model versions using SBGN.



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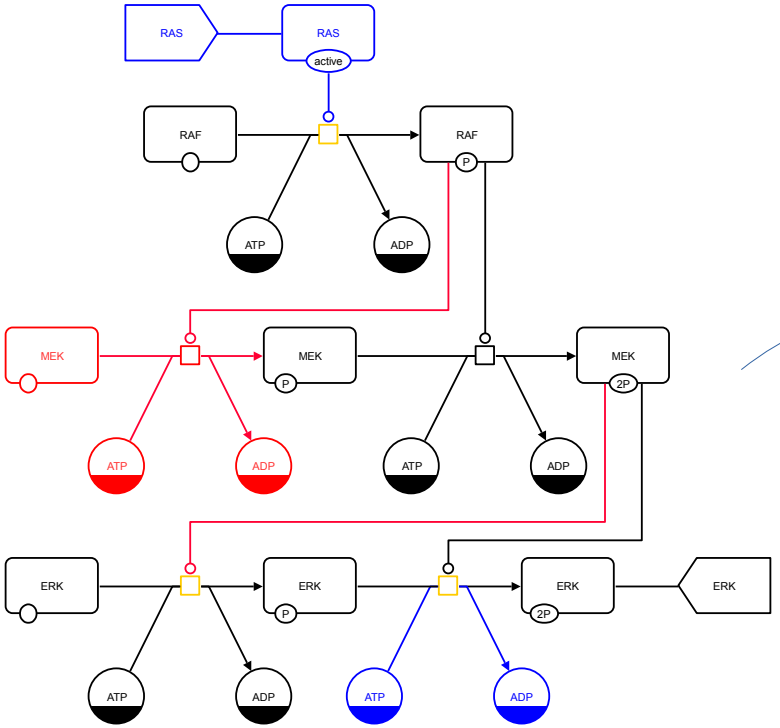
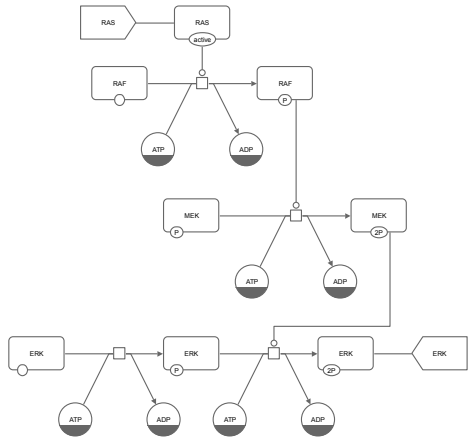


Transition version



Version 2

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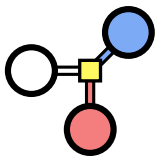
What are the steps?

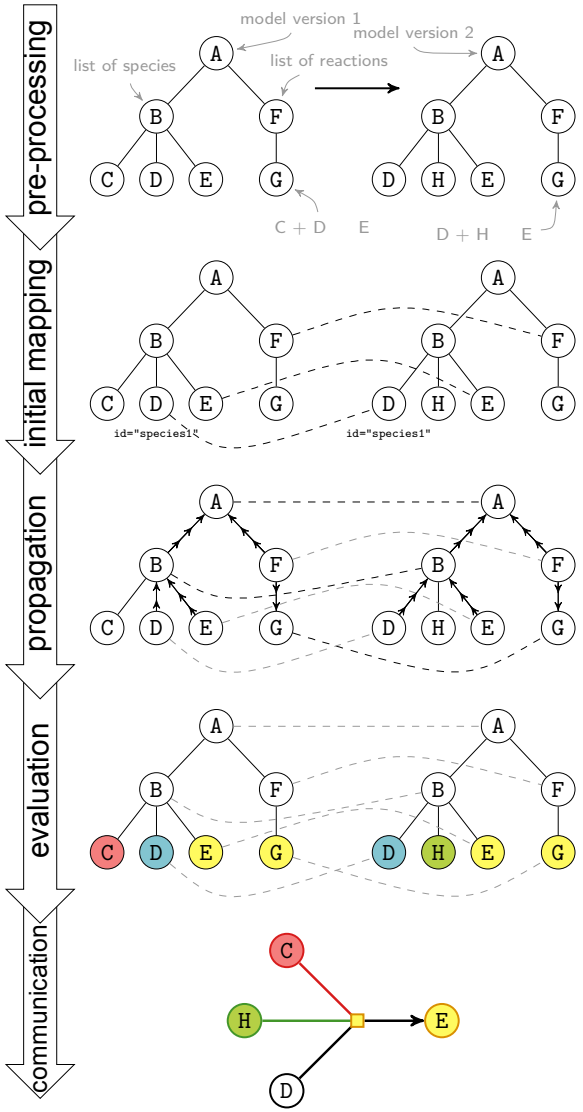
1) Generate a tool to compare differences between two versions

Biochemical Model **Ve**rsion Control **S**ystem



The description of a model's evolution is performed by the BiVeS library.

http://bives.sems.uni-rostock.de

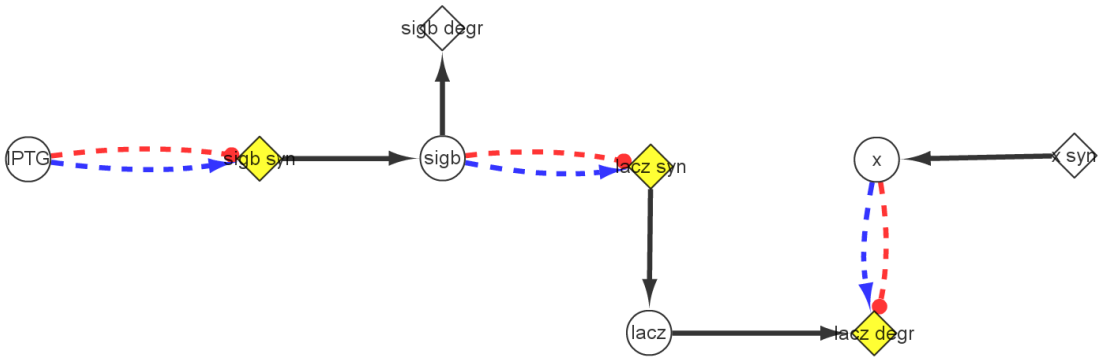


What are the steps?

1) Generate a tool to compare differences between two versions
2) Generate a visual of the differences

Differences are colour coded:

modifications
inserts
deletes



http://budhat.sems.uni-rostock.de

U. Liebal - "Proteolysis of beta-galactosidase following SigmaB activation in Bacillus subtilis" (Mol. BioSyst)
Model Versions: laczsynth-2012-11-10 and laczsynth-2012-11-11

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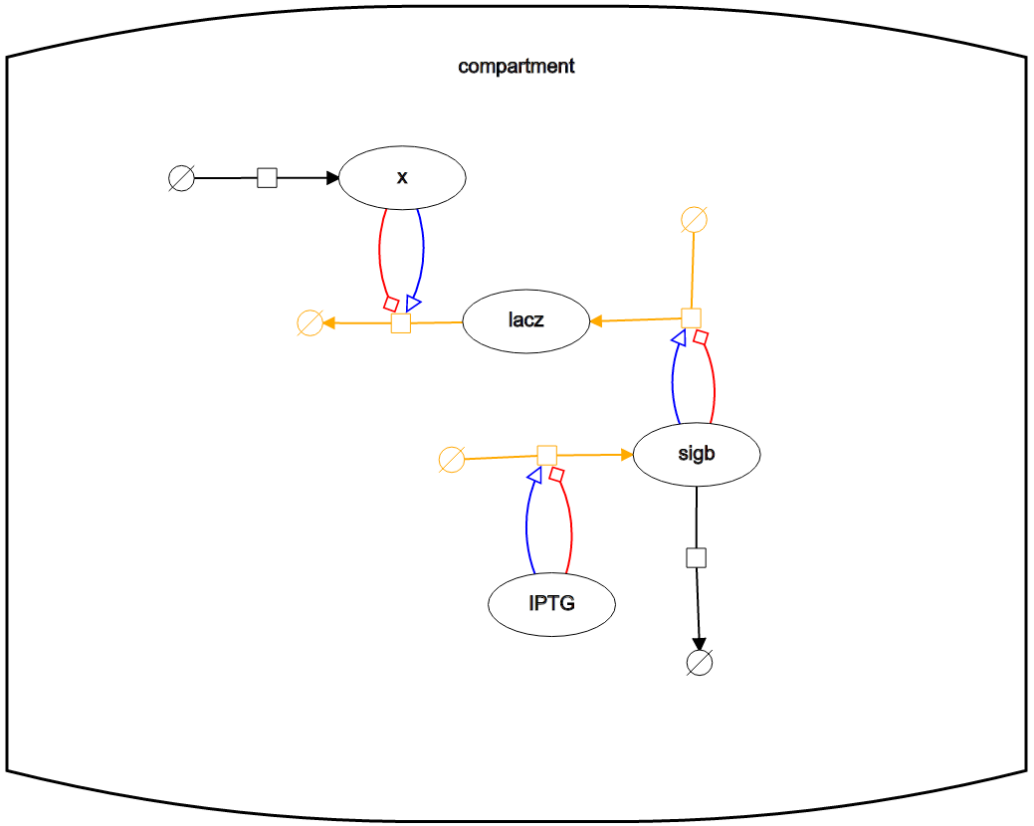
What are the steps?

1) Generate a tool to compare differences between two versions
2) Generate a visual of the differences
3) Make the visual SBGN-compliant

Differences **Vi**sua**L**ization

https://github.com/Gebbi8/DiVil



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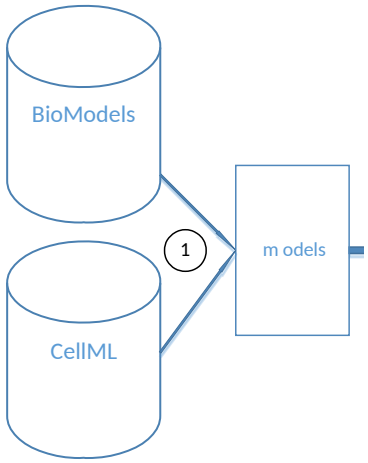
Preliminary workflow



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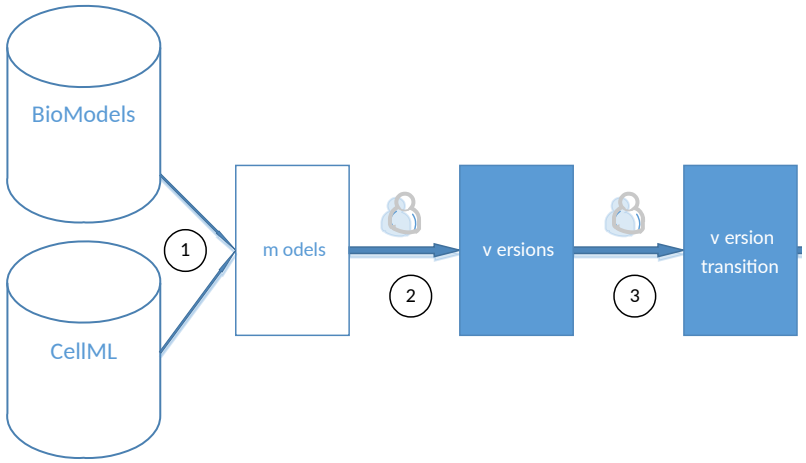

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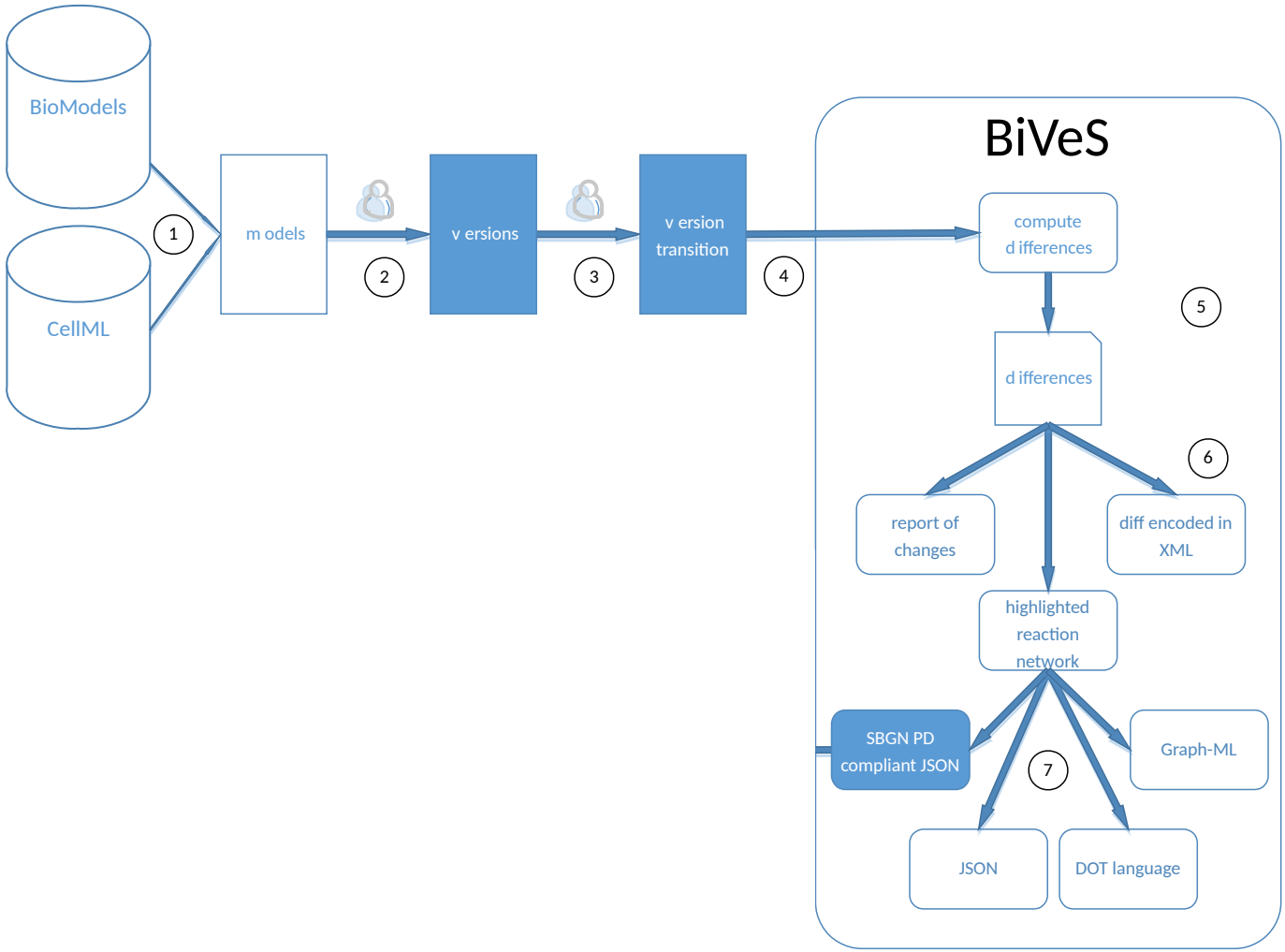

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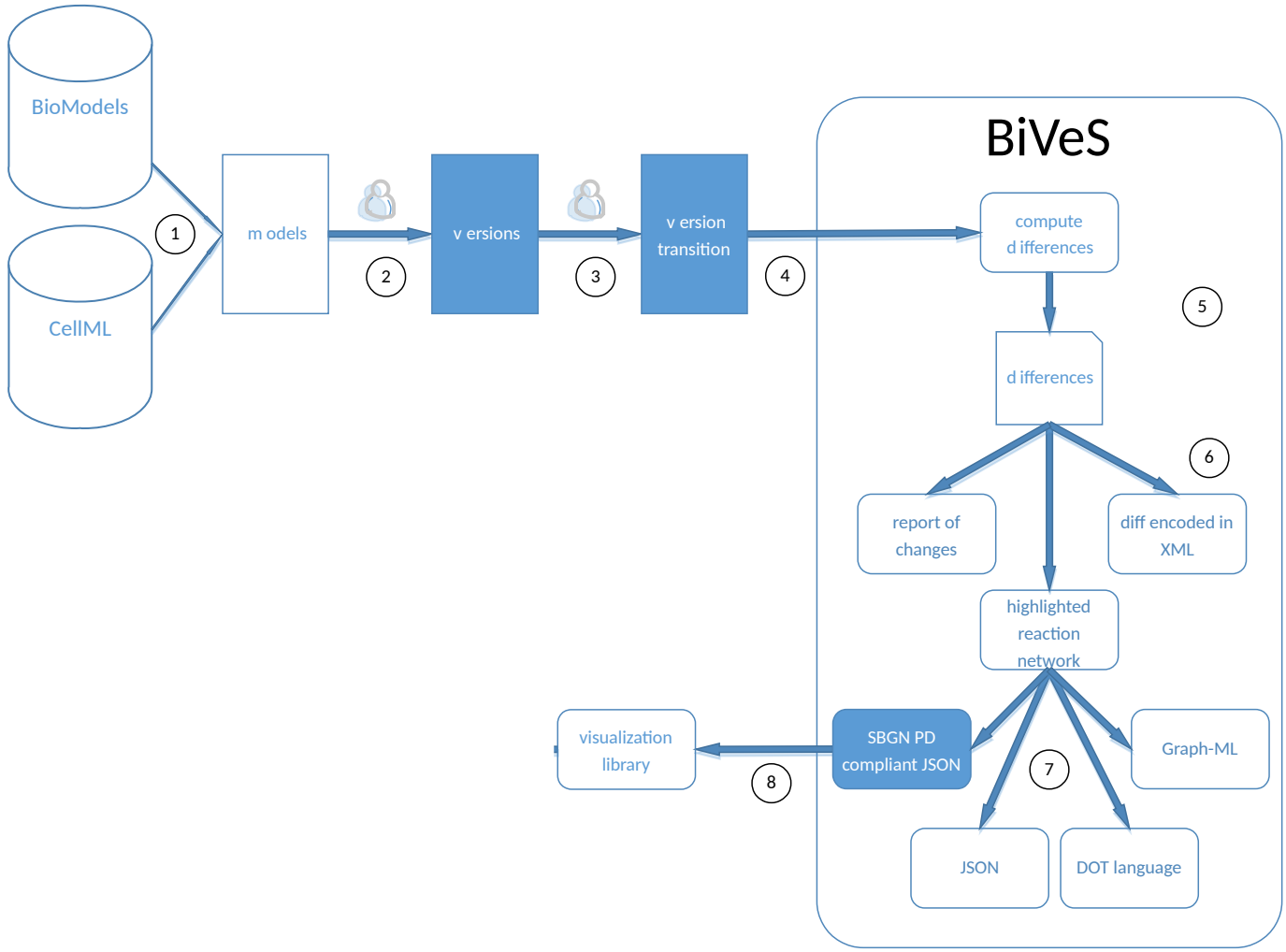
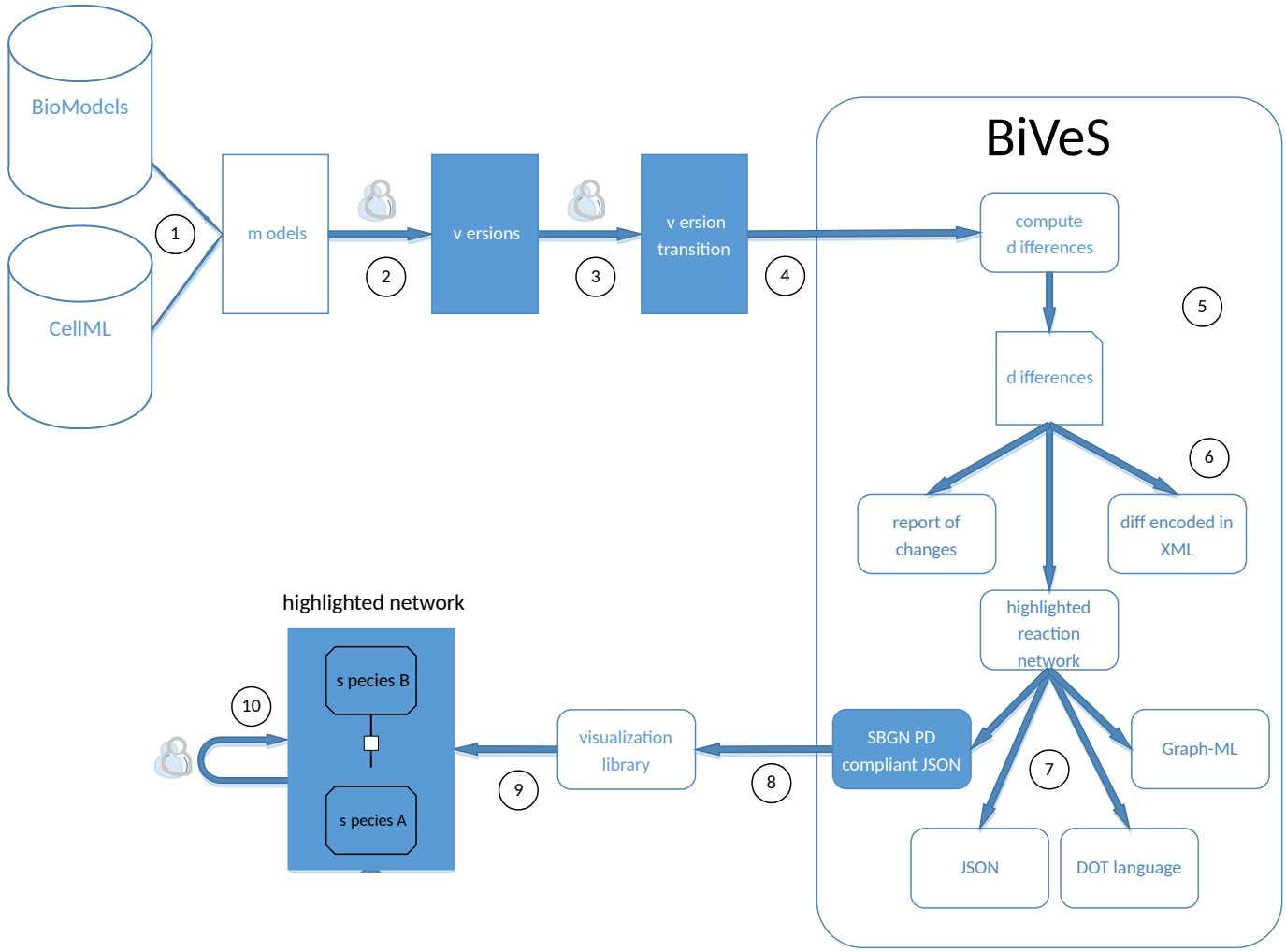


Preliminary workflow



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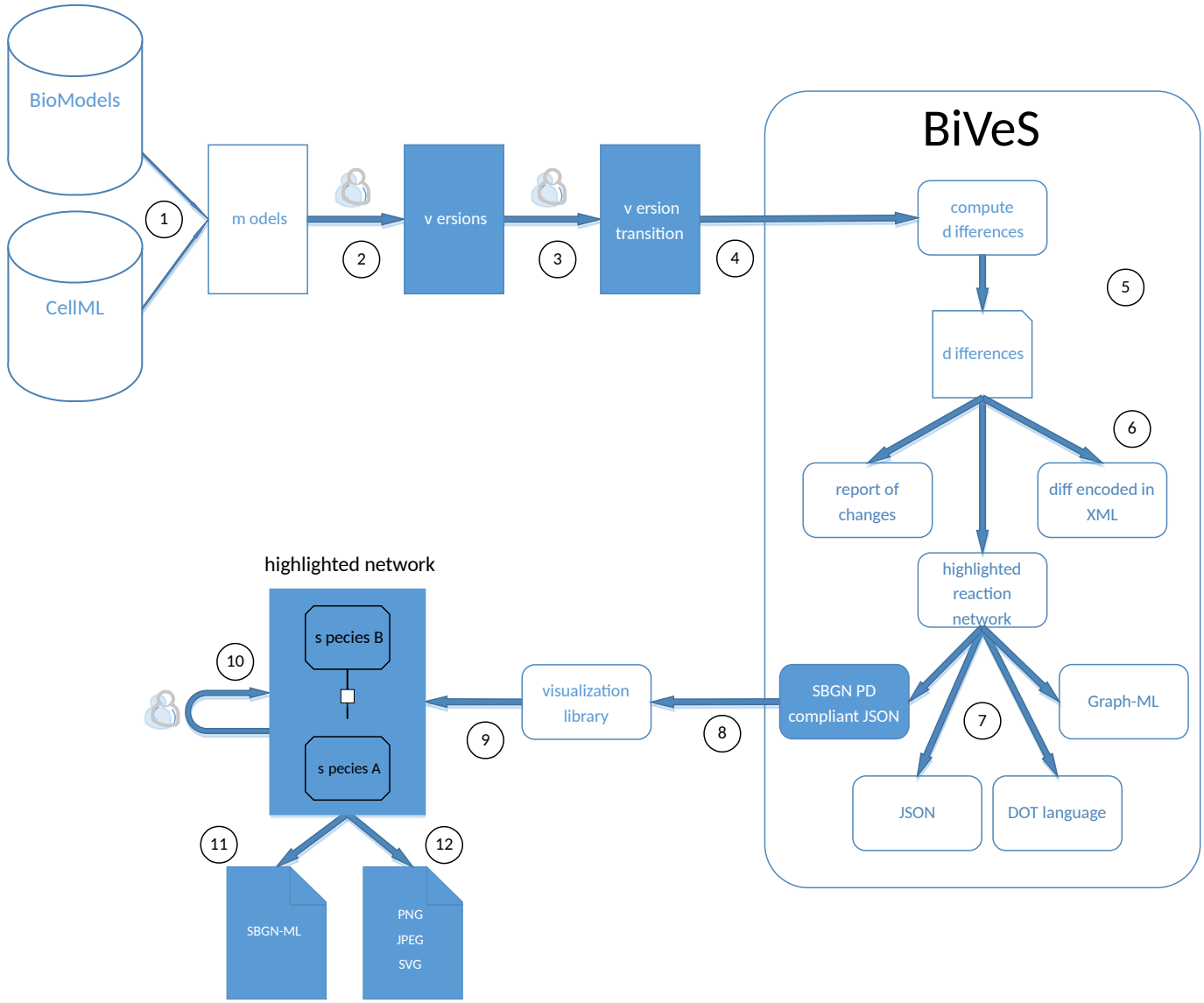
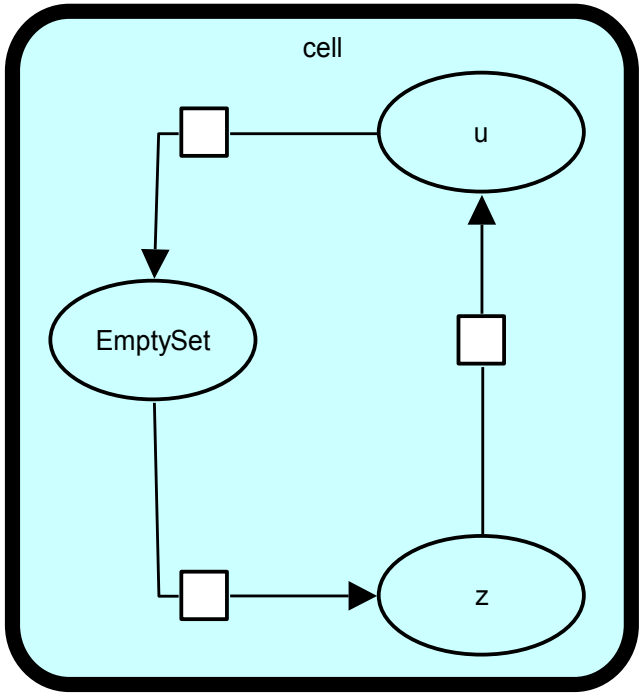
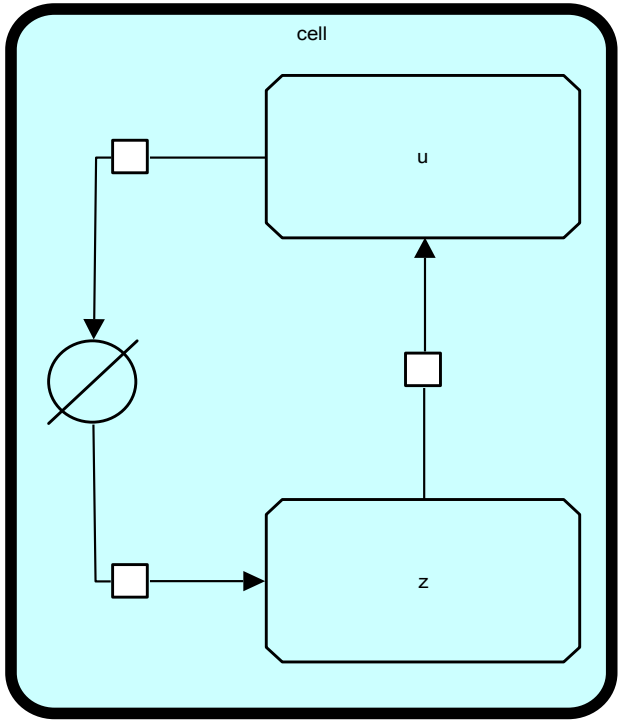


Importance of SBO terms



without SBO terms



with SBO terms

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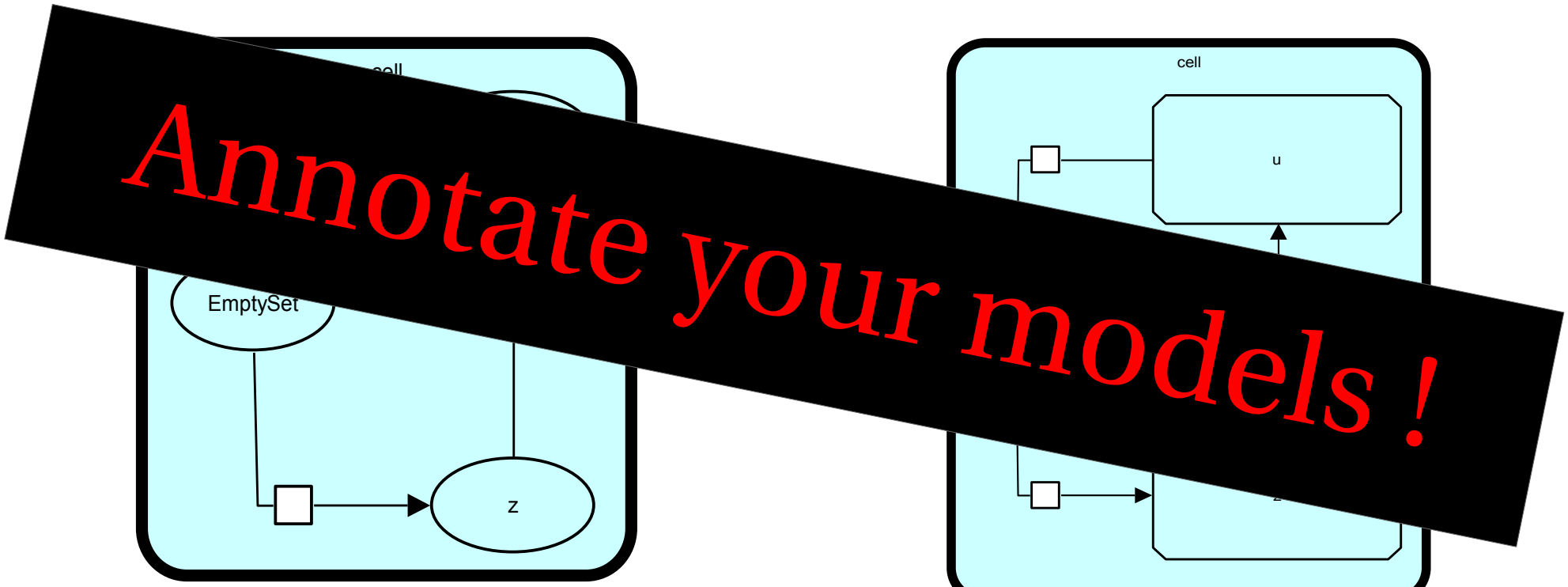

without SBO terms

with SBO terms

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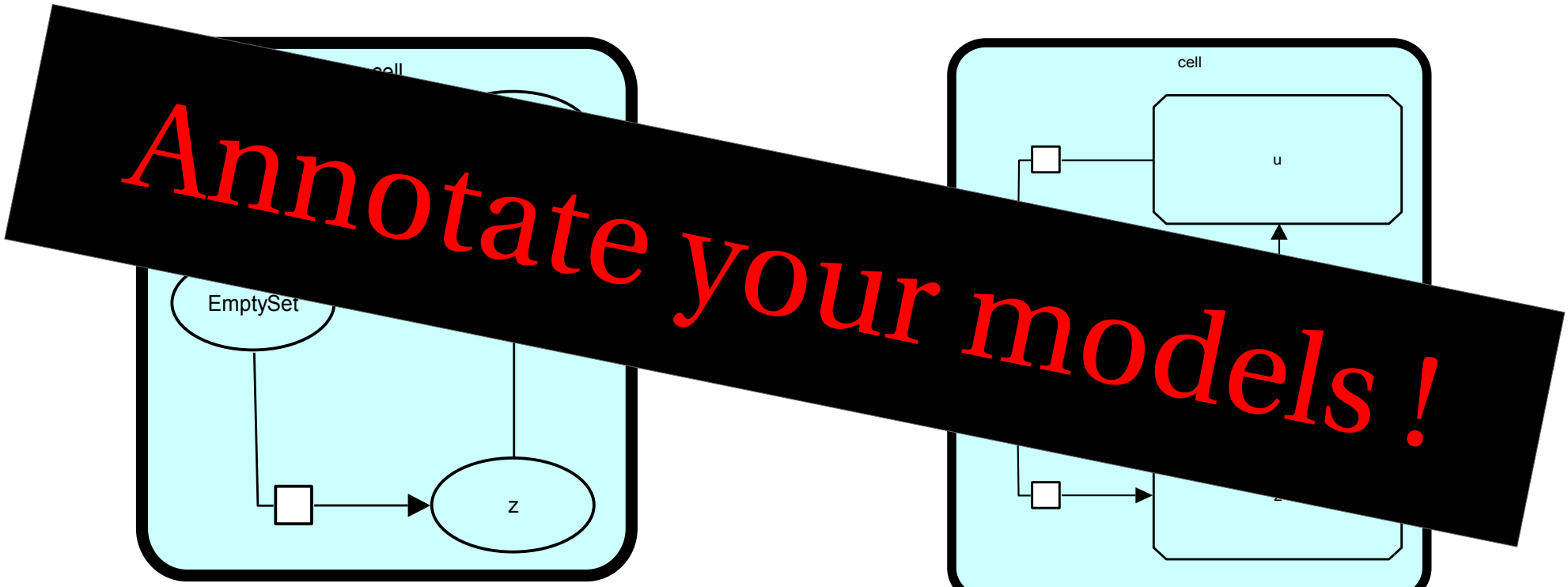
Importance of SBO terms



without SBO terms

with SBO terms

SBGN workshop: still time to join us!

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Conclusion

Prototype: SBGN map showing differences between model versions

- Extension of BiVeS library → information for generating SBGN map
- Automatic force-based layout
- Generation of an SBGN-ML file and graphical exports

Necessary improvements:

- The SBGN output
- Colour information
- User interface

Opportunity for a student internship in Rostock (2-4 months project)
More information: www.sems.uni-rostock.de

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Thank you for your attention!

Tom Gebhardt
DiViL

Martin Scharm
BiVeS and Budhat

The SEMS team

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Bundesministerium für Bildung und Forschung

Projektträger Jülich Forschungszentrum Jülich

Contact: vasundra.toure@uni-rostock.de