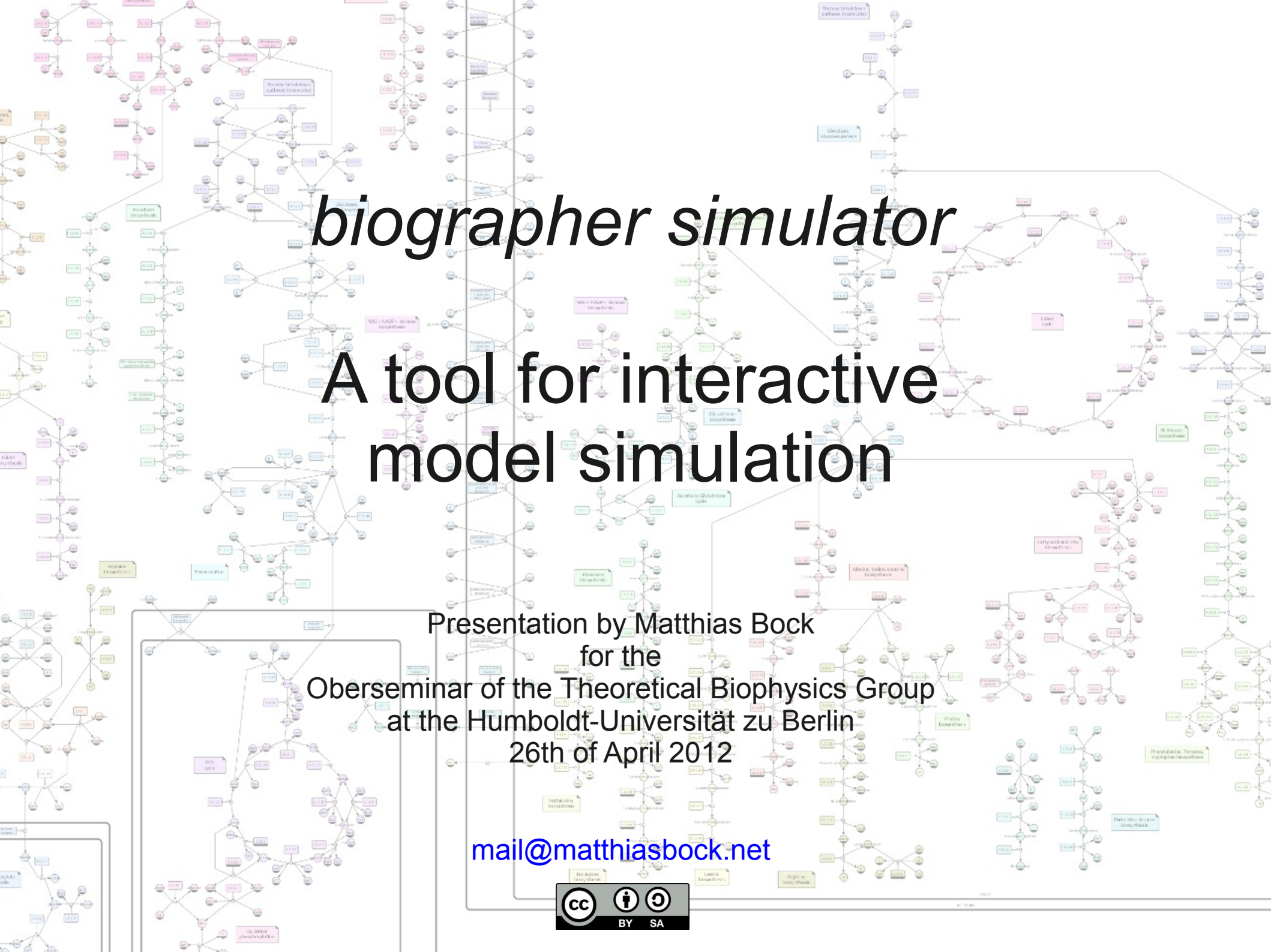


biographer simulator

A tool for interactive model simulation

Presentation by Matthias Bock
for the
Oberseminar of the Theoretical Biophysics Group
at the Humboldt-Universität zu Berlin
26th of April 2012

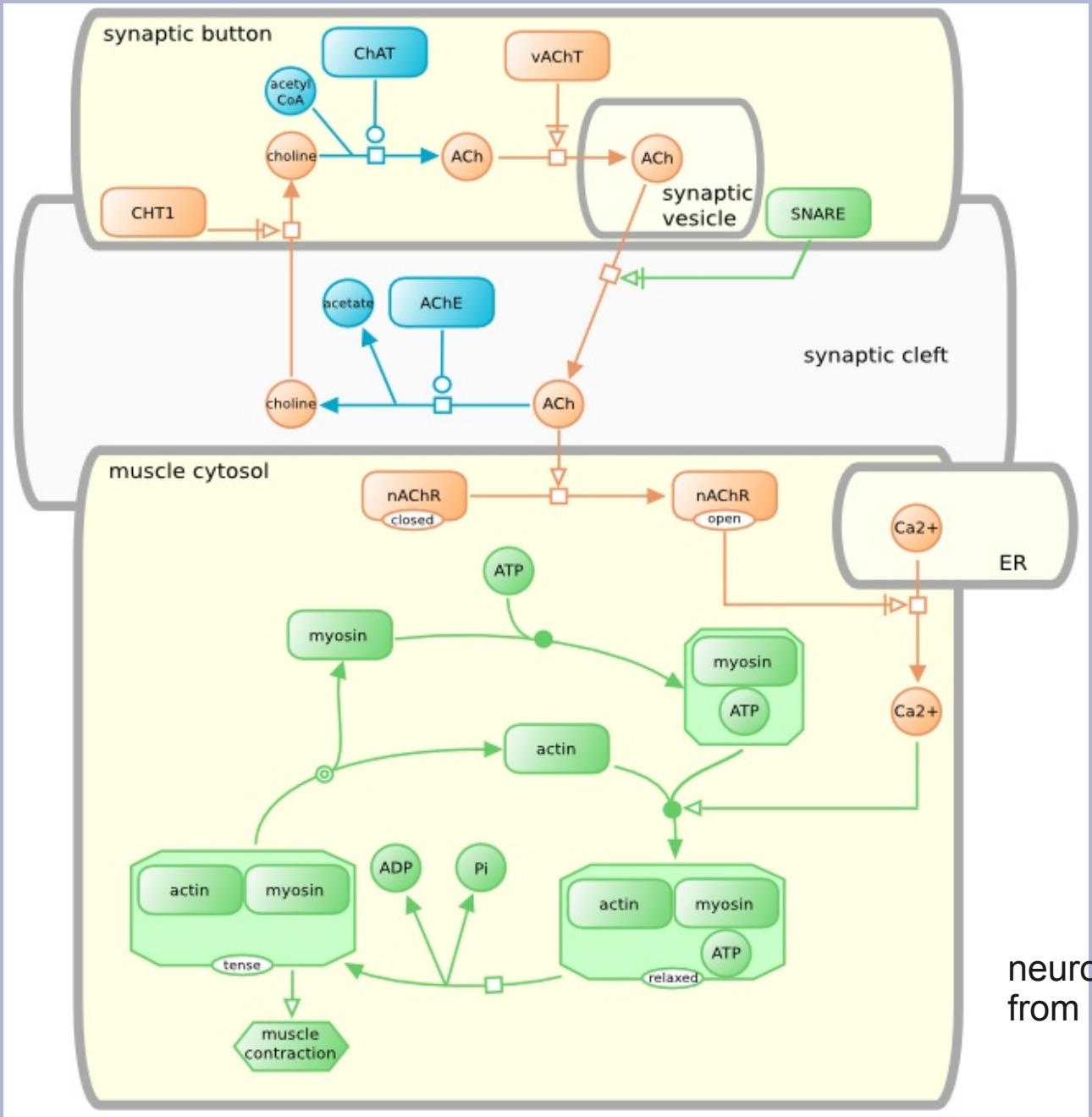
mail@matthiasbock.net

biographer

Systems Biologists want
meaningful visualizations!

SBGN = Systems Biology Graphical Notation
http://SBNG.org/

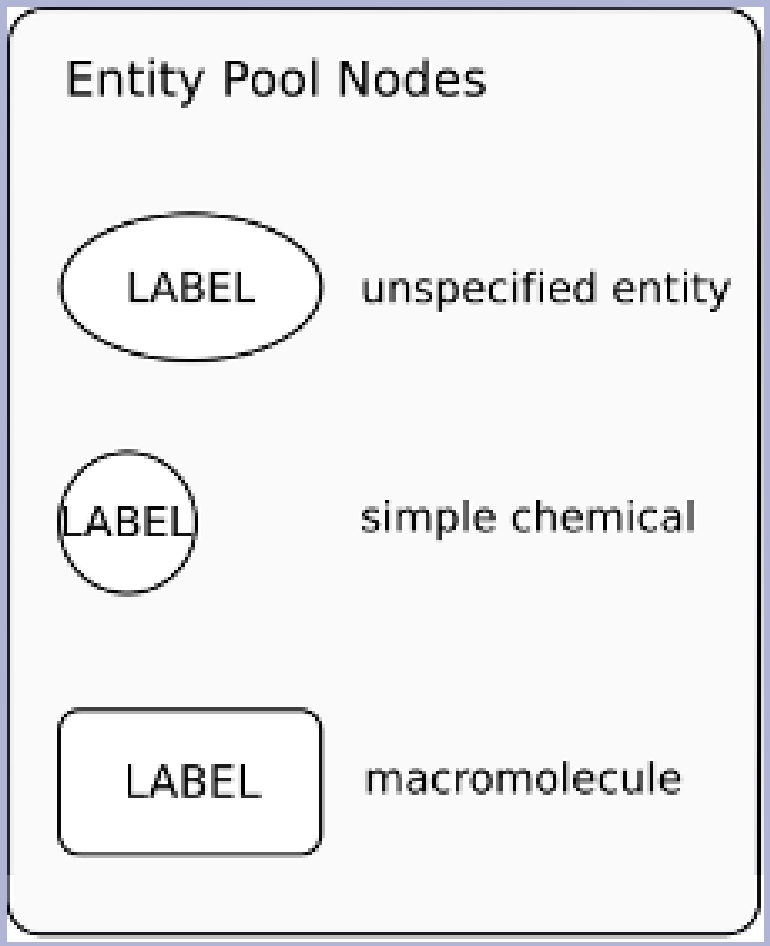
SBGN

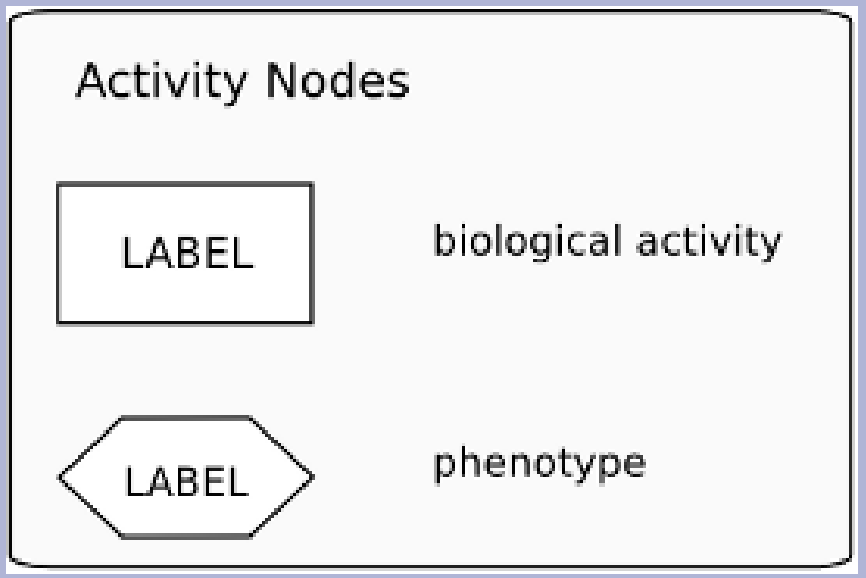


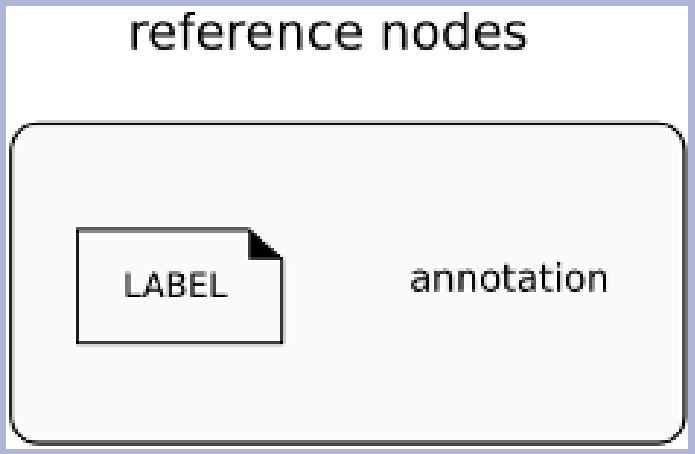
SBGN standardizes, how nodes in a model are supposed to look like

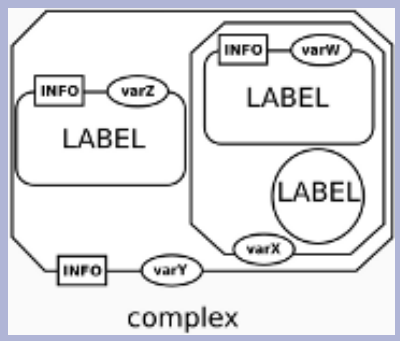
neuro-muscular junction
from http://sbgn.org/

SBGN


Entity Pool Nodes
LABEL
unspecified entity
LABEL
simple chemical
LABEL
macromolecule

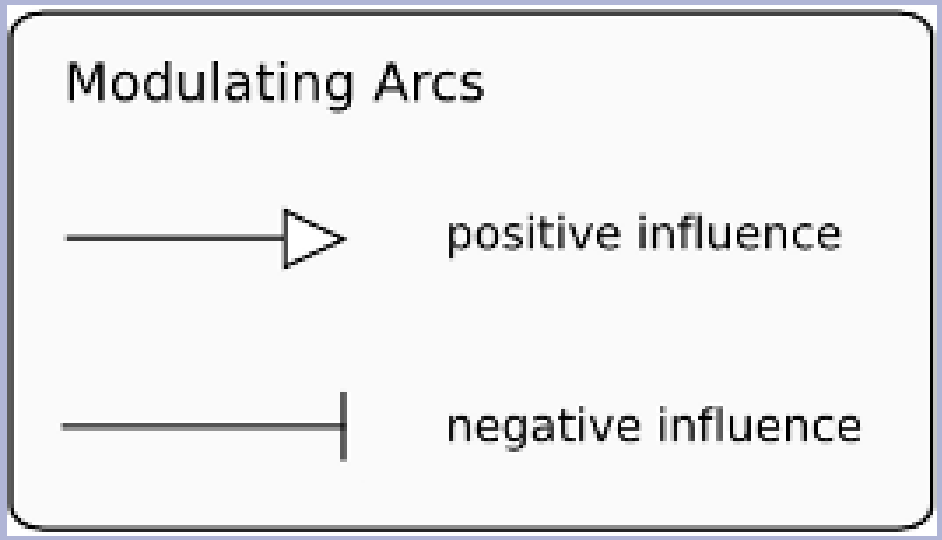

Activity Nodes
LABEL
biological activity
LABEL
phenotype

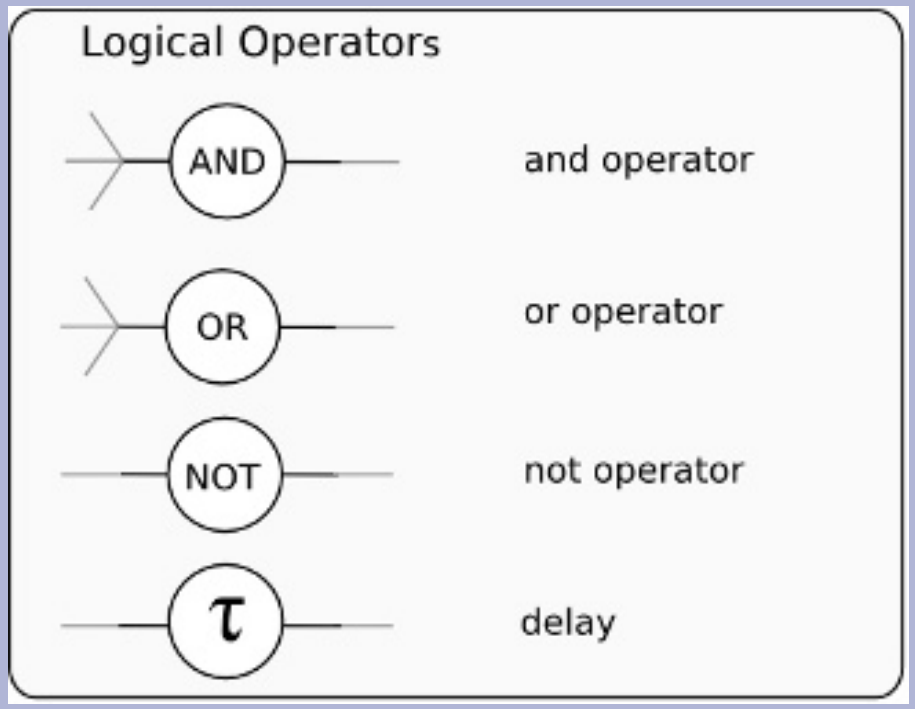

reference nodes
LABEL
annotation


INFO
varZ
LABEL
INFO
varW
LABEL
LABEL
varX
INFO
varY
complex

SBGN

and not only nodes, but also: interactions





this brought me to the idea ....

The challenge

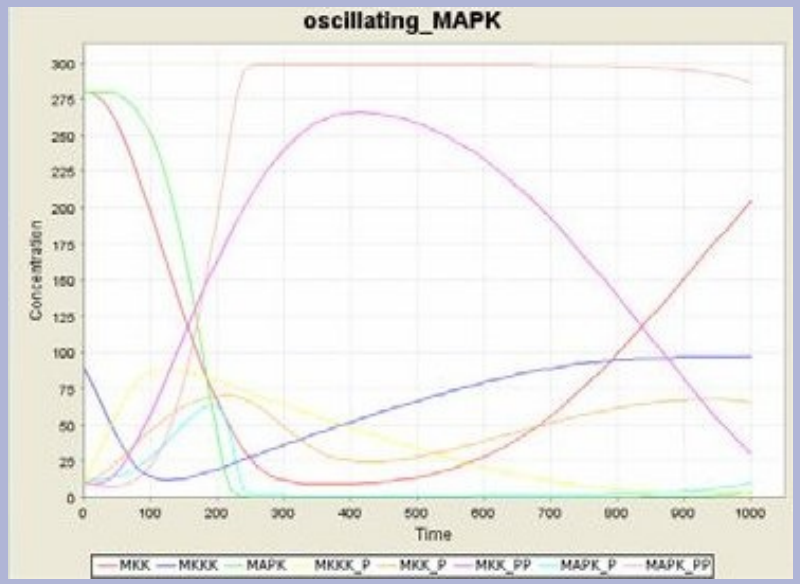
„bringing life to modelled life“

visualize the network's activity state
inside it's SBGN illustration

bringing together modelling and testing

Theoretical models

1. model kinetics using equations:
   * Copasi



Oscillating MAPK network
from CellDesigner Online Help

2. model as Boole'an network using logical expressions:
   * R
   * BooleNet

BooleNet

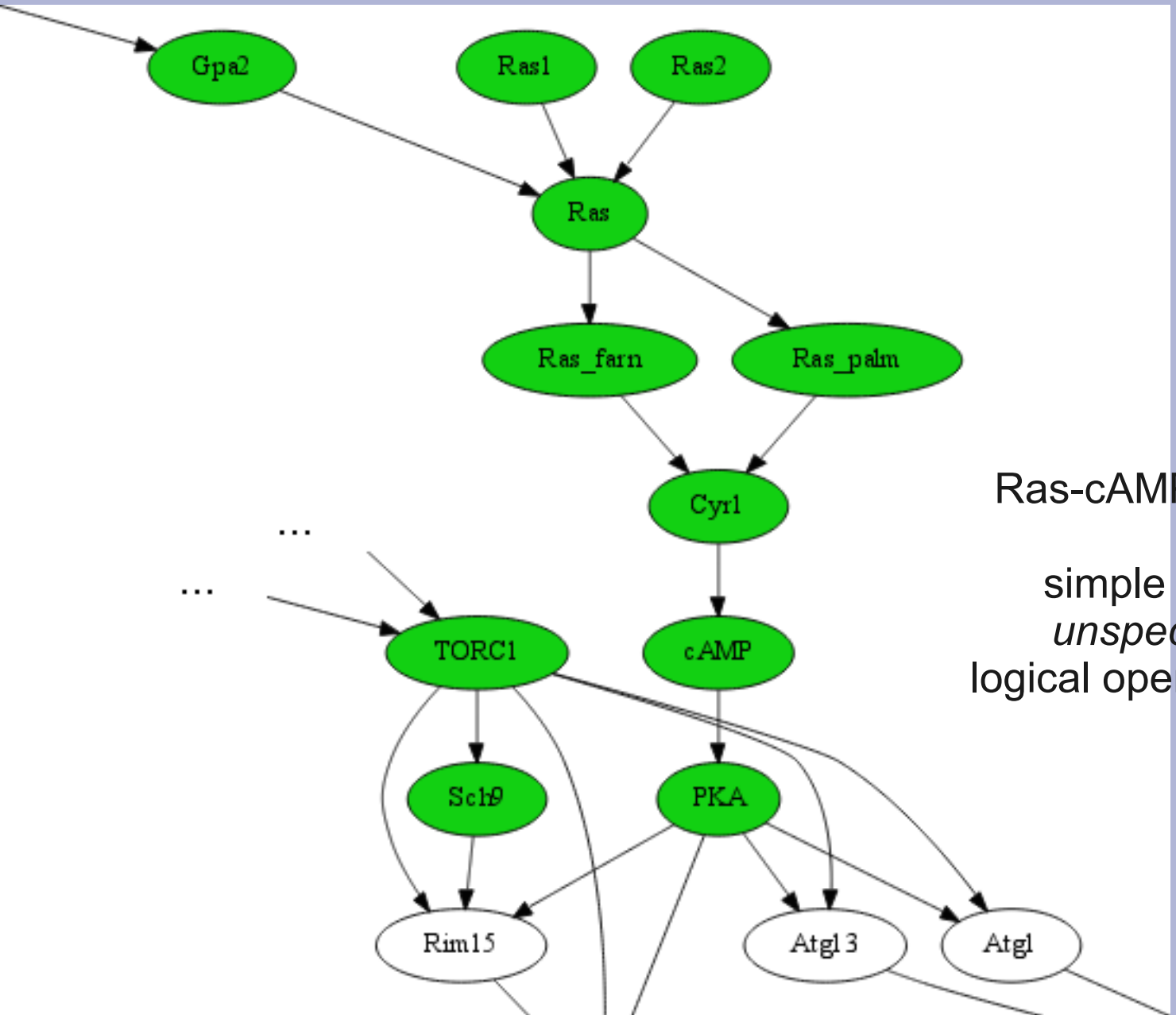
BooleNet Python library:

* completely open-source
* runs platform-independent
* established solution for Boole'an network analysis
* enables extraordinary quick and easy modelling

model = file of Update Rules
e.g.

```
# my example BooleNet model
Ras* = Glucose and GlucoseReceptor and (not Inhibitor)
```

Visualization



Ras-cAMP-PKA pathway

simple rendering as
unspecified nodes;
logical operators not shown

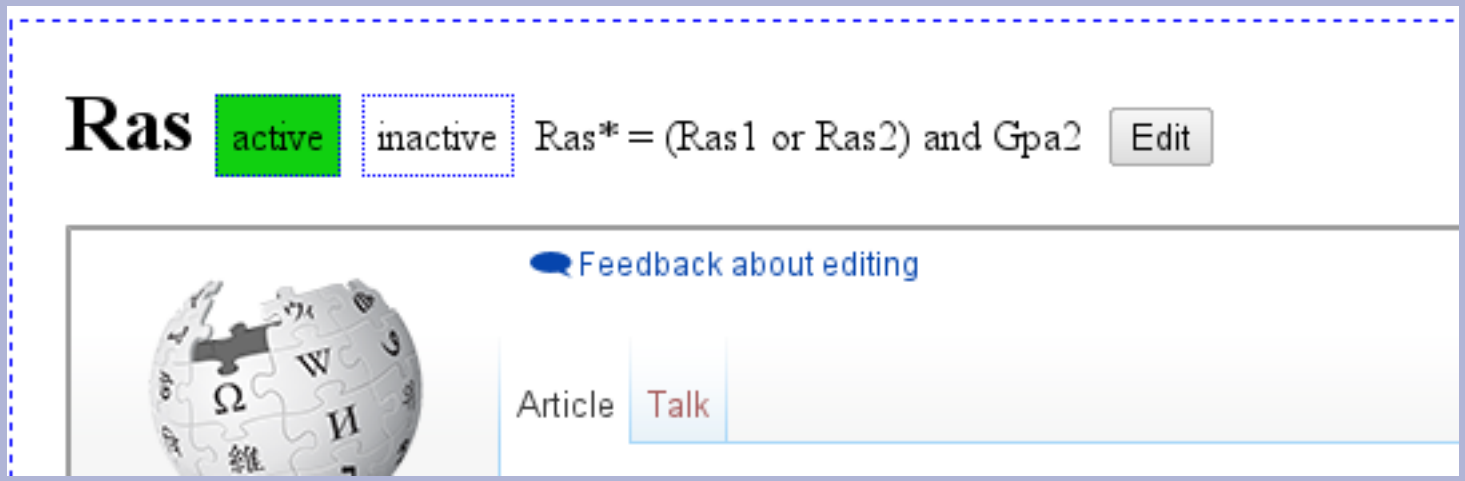
Interactivity

* click to simulate

* watch the progression of acitivitiy changes inside your network in „real time“

* click to see node annotation

* in-browser logic editor



State characterization

isn't simulation only with 0s and 1s kind of a too simple approach ?

State characterization

isn't simulation only with 0s and 1s kind of a too simple approach ?

present/absent

active/inactive

phosphorylated/dephosphorylated

complexed/dissociated

receptor firing/off

gene transcription/silent

State characterization

isn't simulation only with 0s and 1s kind of a too simple approach ?

present/absent

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receptor firing/off

gene transcription/silent

 # States of Glucose: True="present", False="absent"

Annotations

1. single nodes

included via Python comment „*# Annotation of ...*“

e.g.

```
...
Glucose* = not metabolism
# Annotation of Glucose: „my energy source“
...
```

2. whole pathway

via SBGN labels

Demonstration ...

Future aims

allow offline usage

SBML import/export

automated model generation

update rules controlling other node properties, e.g. localization

full SBGN conformity

in-browser modelling

different layouting possibilities

and fancy tablet support
(touch gestures: slide, zoom, node drag'n'drop)

Future aims

will be addressed in ...

http://code.google.com/p/biographer/wiki/Simulator

Thank you very much
for your attention!