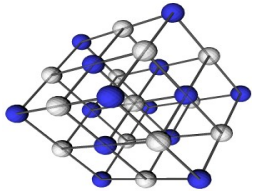
SBGN support in BIOCHAM

Biochemical Abstract Machine



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SBGN-6, COMBINE MEETING, Edinburgh UK

SBGN support in BIOCHAM

Outline:

- ***BioCham* – Biochemical Abstract Machine**
- ***SBGN* support in BioCham**
- **Biocham Reaction Graph *Editor***
- **Conclusion**
- **On-going work**

SBGN support in BIOCHAM

- ***BioCham – Biochemical Abstract Machine*** → *Modelling*, *Analysing*
  - *- http://contraintes.inria.fr/biocham*
  - ***- different simulators***
  - ***- temporal logic based language***
  - ***- features for correcting/completing/reducing/relating/coupling models***

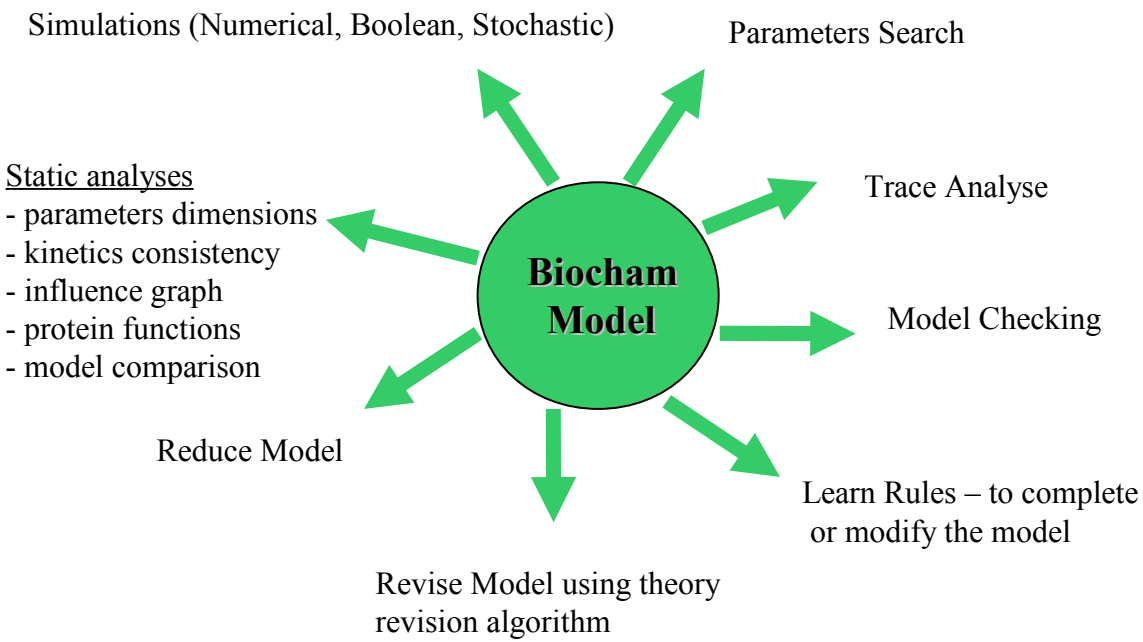
BIOCHAM MODEL Consists of

SBML compatible

- Rules
- Events
- Initial concentrations
- Molecules
- Compartments volumes
- Parameters
- Macros
- *Conservations Laws*
- *Temporal Logic Specifications*

SBGN support in BIOCHAM

- ***Analysing features in Biocham:***



SBGN support in BIOCHAM

- ***SBGN Entity pool nodes, Defined Sets of EPNs and Auxiliary Units:***

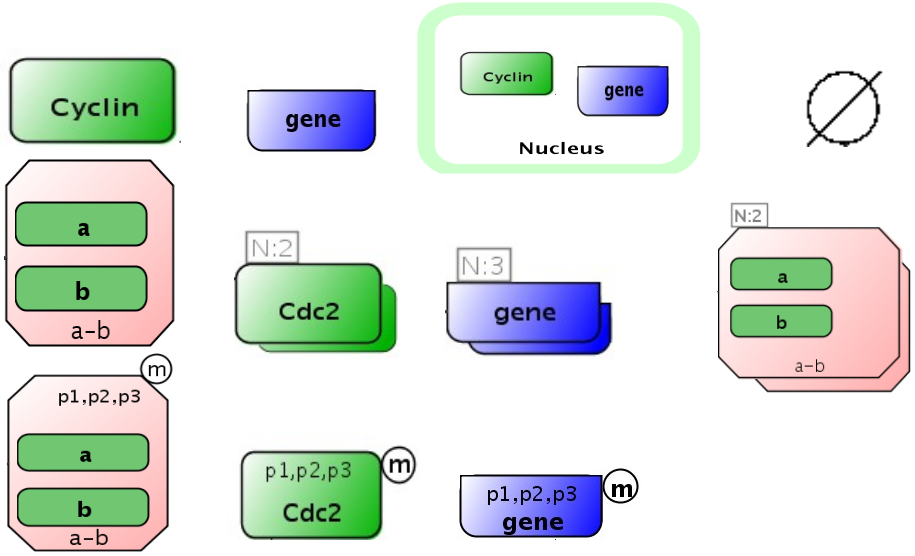
Macromolecule, Nucleic Acid Feature, Multimer, Complex, Source and Sink, Compartment, Unit of Information(cardinality), State Variable(modified)

Biocham objects' grammar:

object = *molecule* | *molecule::name* located molecule

molecule =
- *name*
- | *molecule-molecule* molecular complex
- | *molecule~{name,...,name}* modified molecule
- | *gene*
- | (*molecule*)

gene = *#name*



SBGN support in BIOCHAM

- ***SBGN Entity pool nodes, Defined Sets of EPNs and Auxiliary Units:***

Macromolecule, Nucleic Acid Feature, Multimer, Complex, Source and Sink, Compartment, Unit of Information(cardinality), State Variable(modified), *Labeled Clone Marker!!!*

Biocham objects' grammar:

object = *molecule* | *molecule::name* located molecule

molecule =

name	
| *molecule-molecule*	molecular complex
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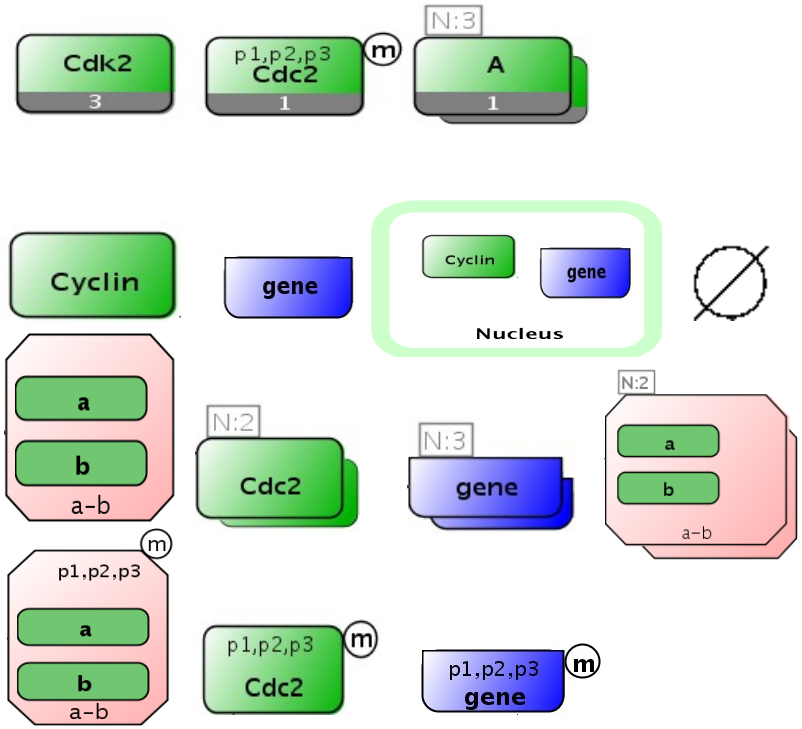


SBGN support in BIOCHAM

- ***SBGN support in BioCham:*** **SBGN Process Nodes :**

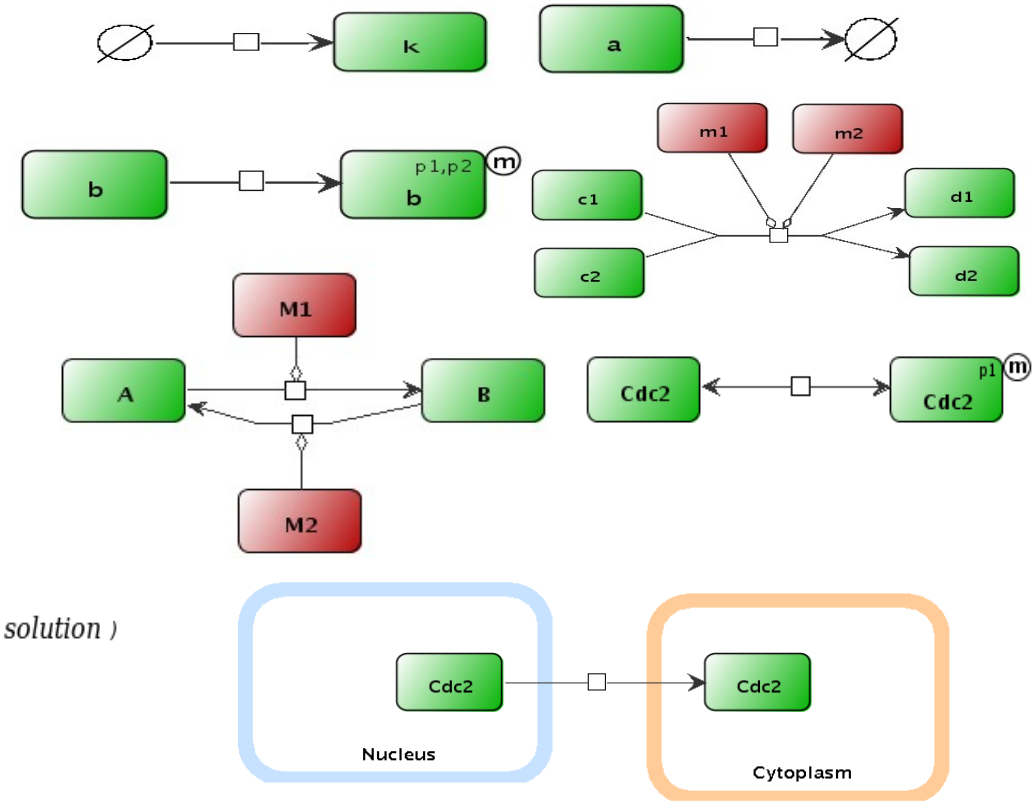
Process, Association and Dissociation

Biocham reactions' grammar:

reaction = *kinetics for basic_reaction*
| *basic_reaction*
| *name : basic_reaction*
| *name : kinetics for basic_reaction*

basic_reaction = *solution => solution.*
| *solution =[object]=> solution.*
| *solution =[solution => solution]=> solution.*
| *solution <=> solution.*
| *solution <=[object]=> solution.*

solution = *_ | object | integer*object | solution + solution | (solution)*



SBGN support in BIOCHAM

- ***SBGN support in BioCham:*** **SBGN Process Nodes and Arcs :**

Process, Association and Dissociation; Consumption, Production and Modulation

Biocham reactions' grammar:

reaction = *kinetics for basic_reaction*
| *basic_reaction*
| *name : basic_reaction*
| *name : kinetics for basic_reaction*

basic_reaction = *solution => solution.*
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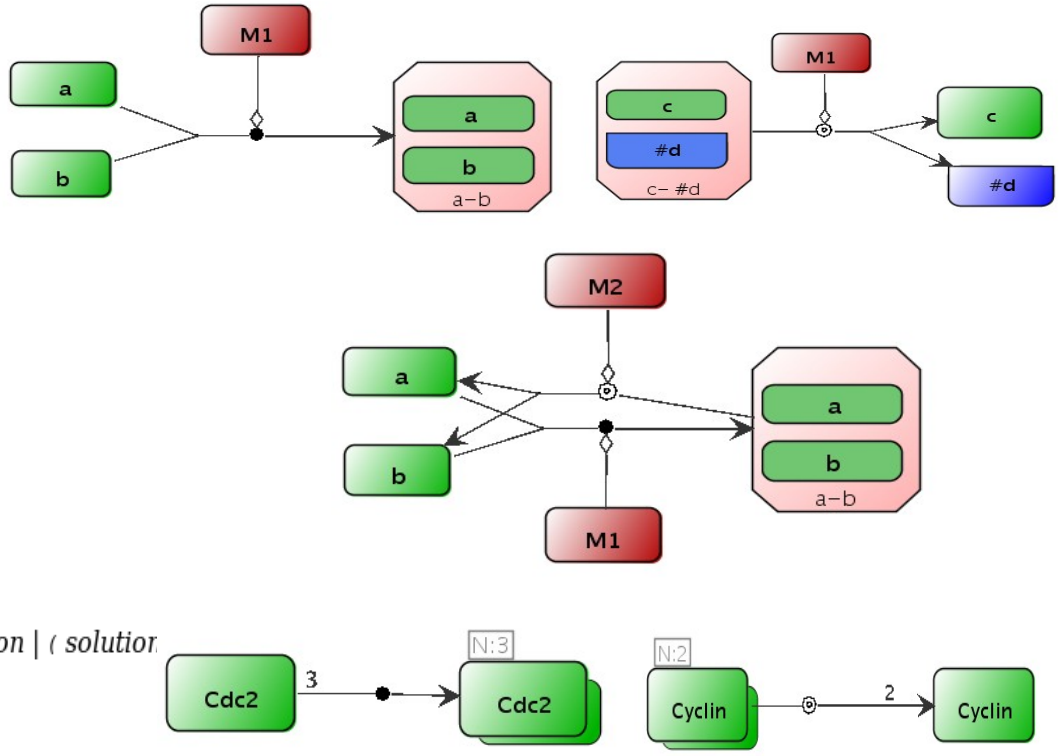
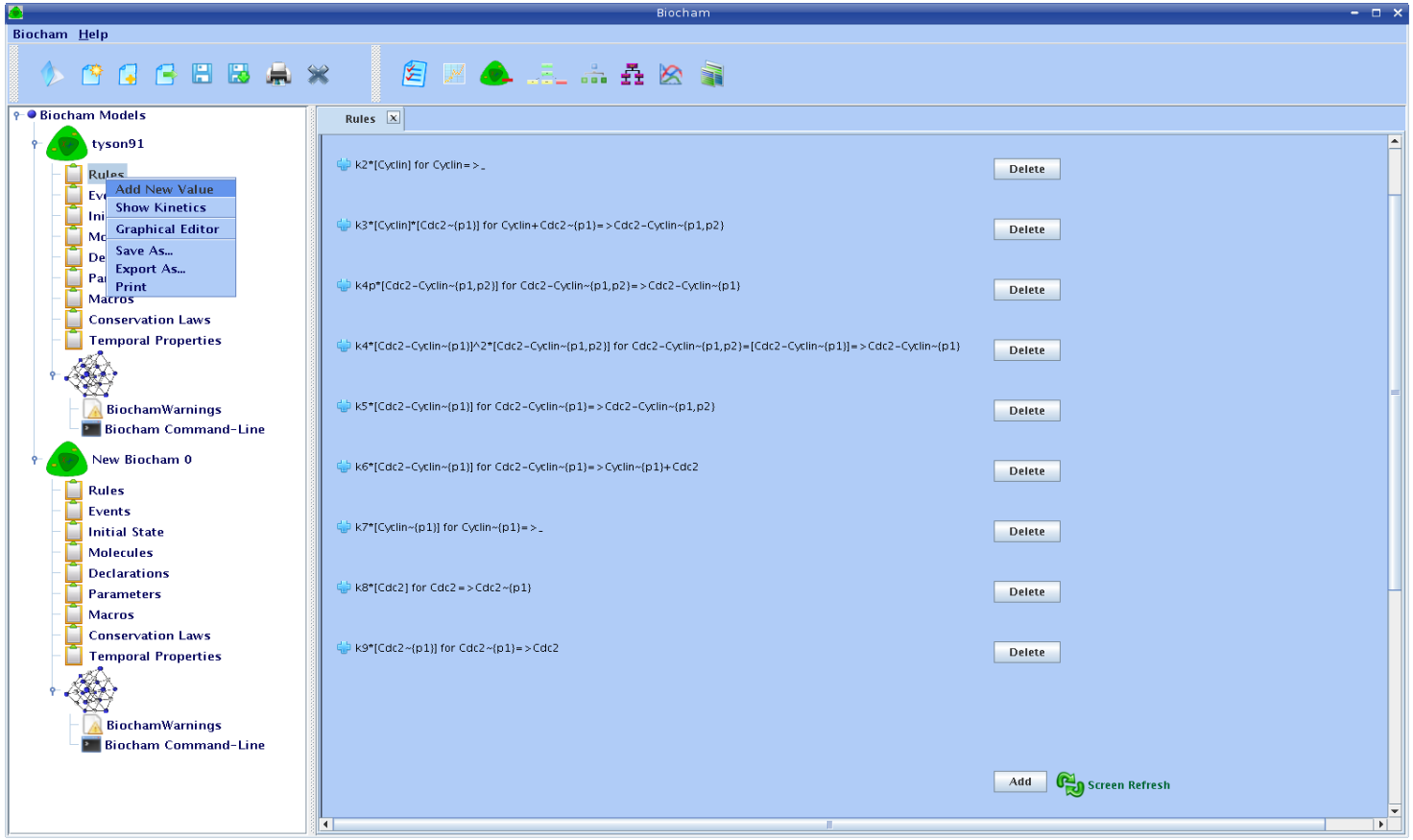
solution = *_ | object | integer*object | solution + solution | (solution*



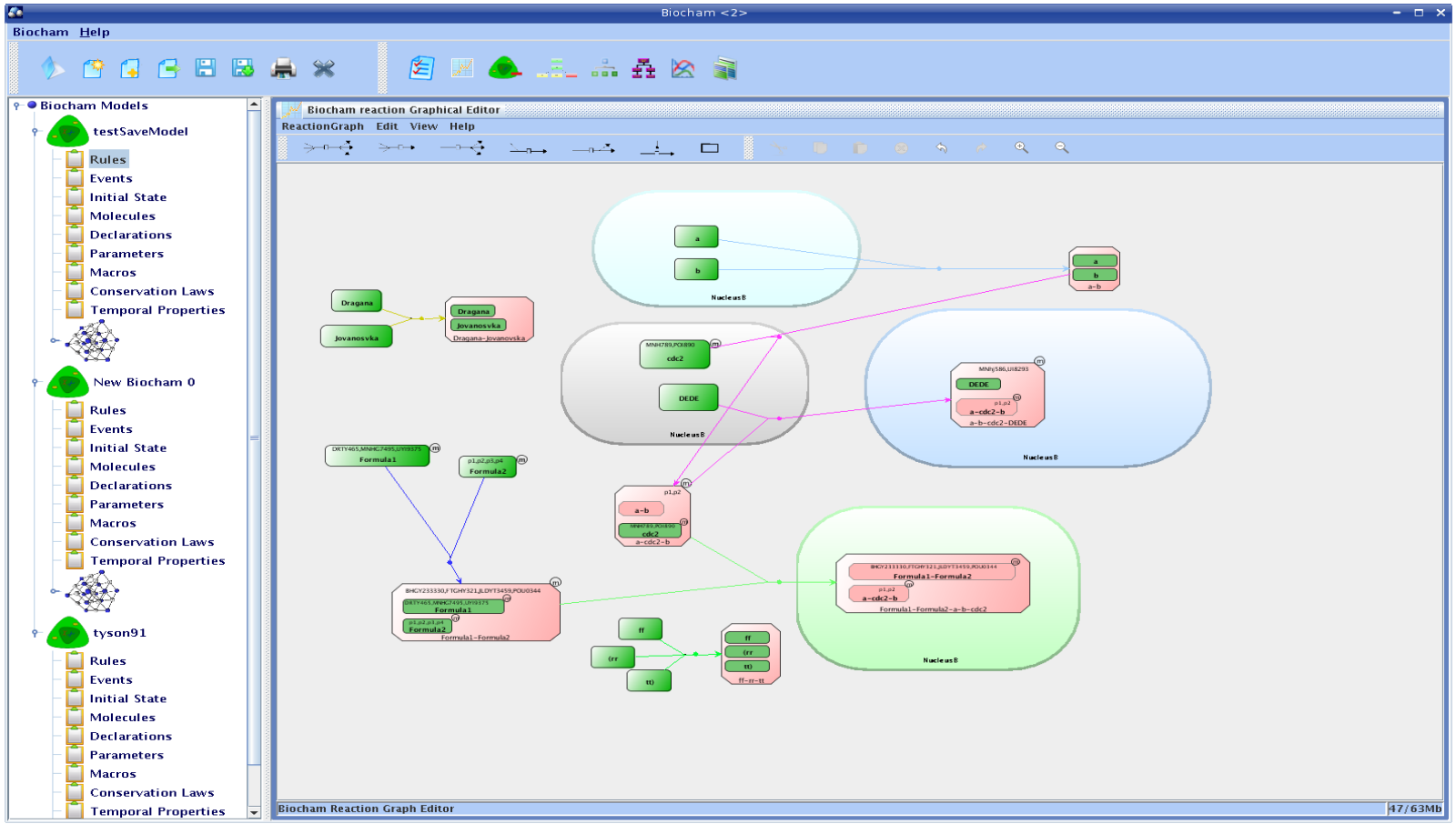
SBGN support in BIOCHAM

- ***Biocham Reaction Graph Editor***



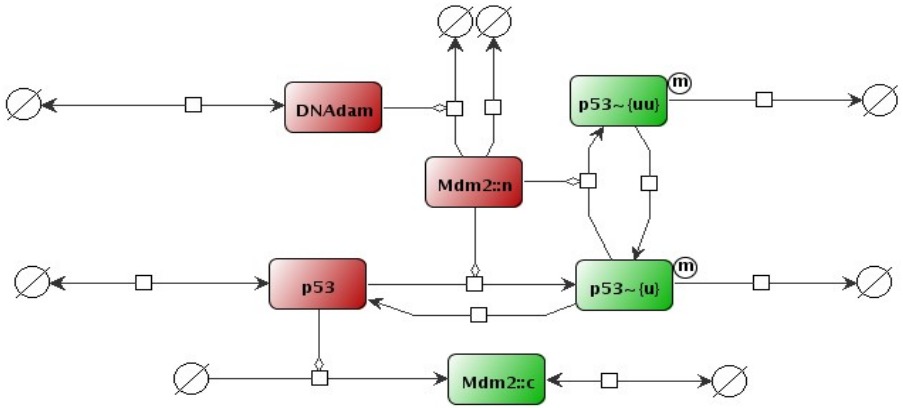
SBGN support in BIOCHAM

- ***Biocham Reaction Graph Editor***



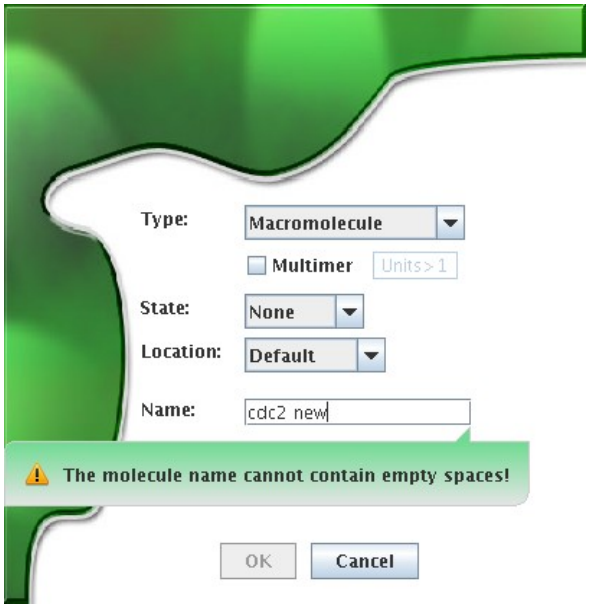
SBGN support in BIOCHAM

- *Biocham Reaction Graph Editor*



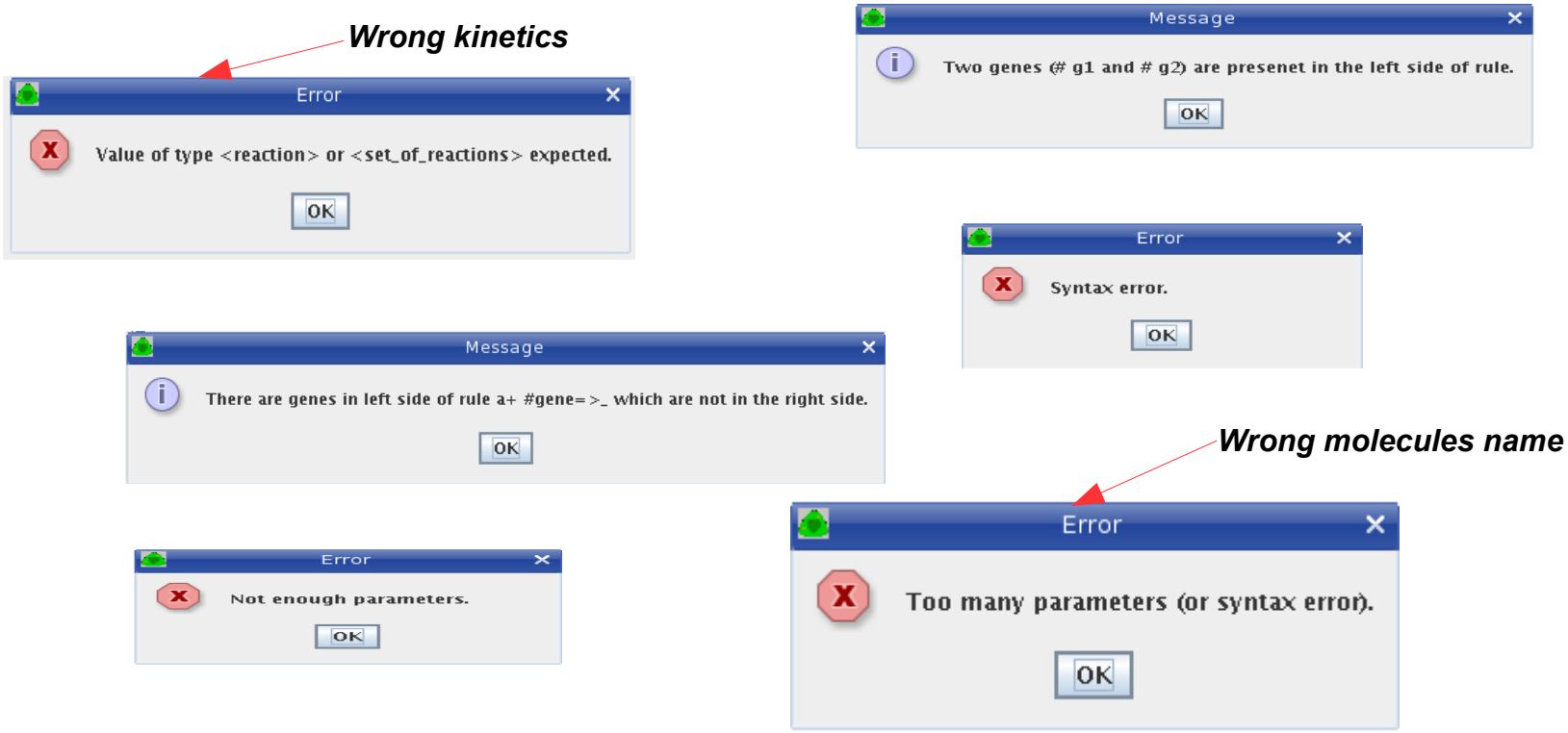
BioCham Reaction Graph Editor

Validation of the syntax and the semantics



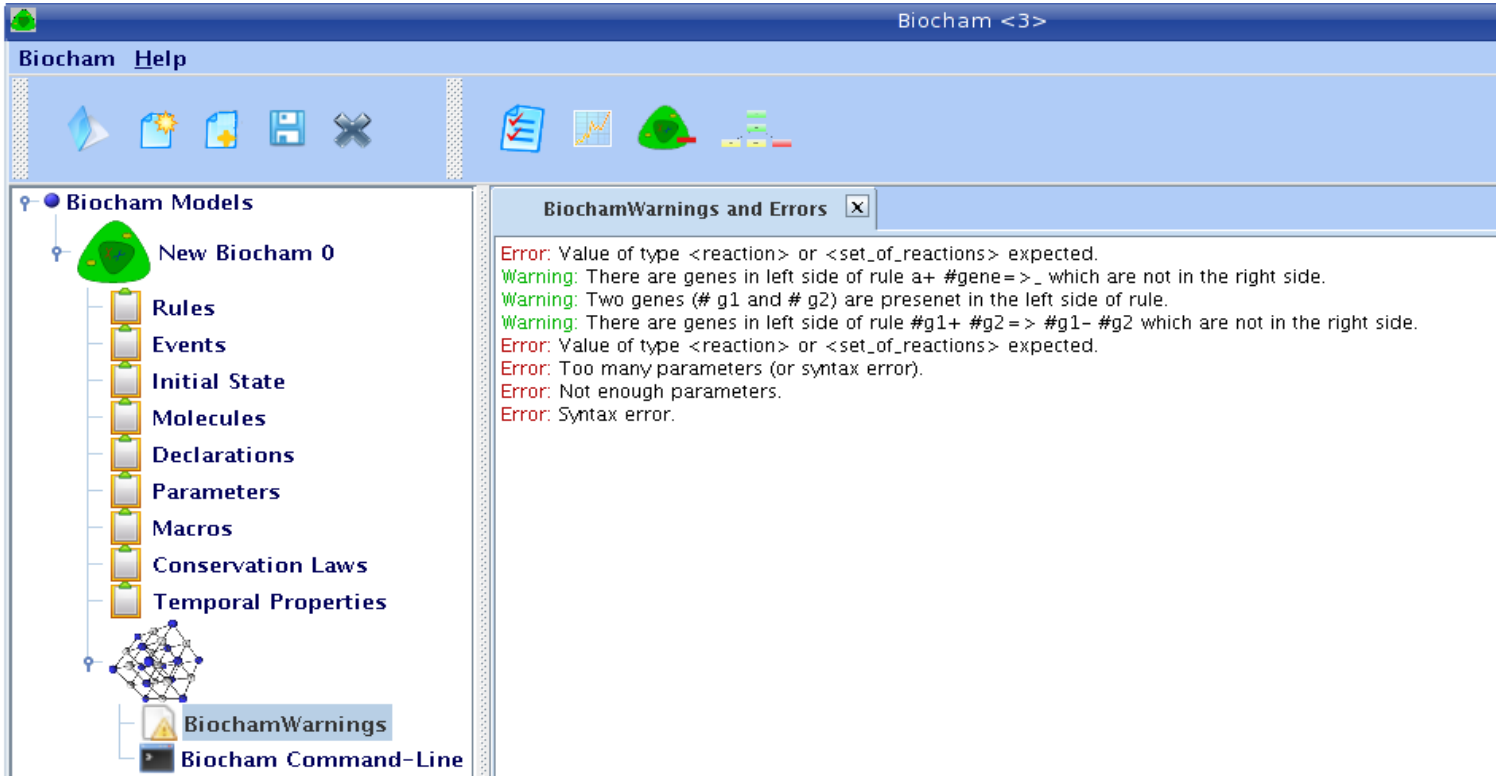
BioCham Reaction Graph Editor

Validation of the syntax and the semantics



BioCham Reaction Graph Editor

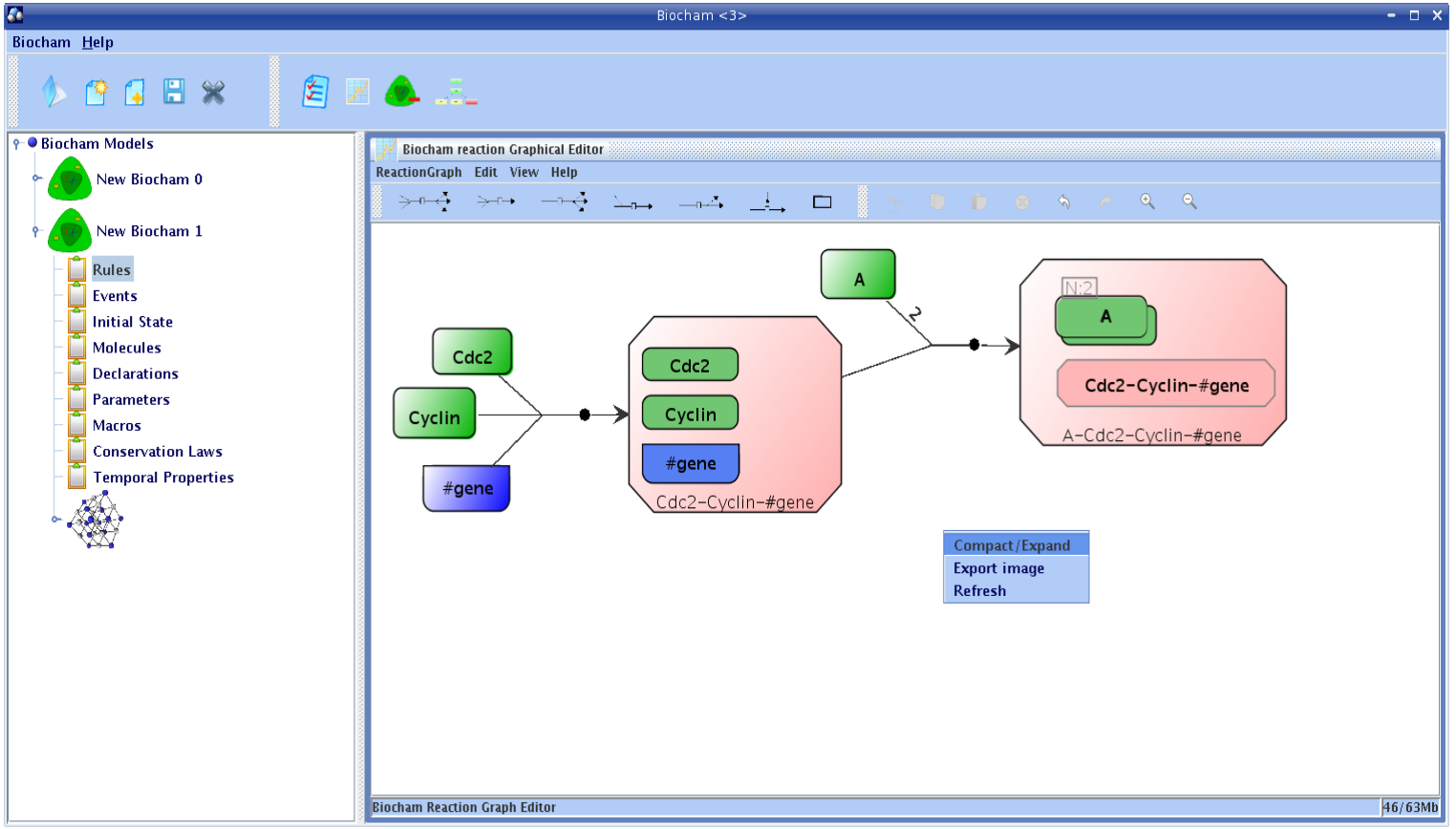
Validation of the syntax and the semantics



CONCLUSION

Proposal for SBGN

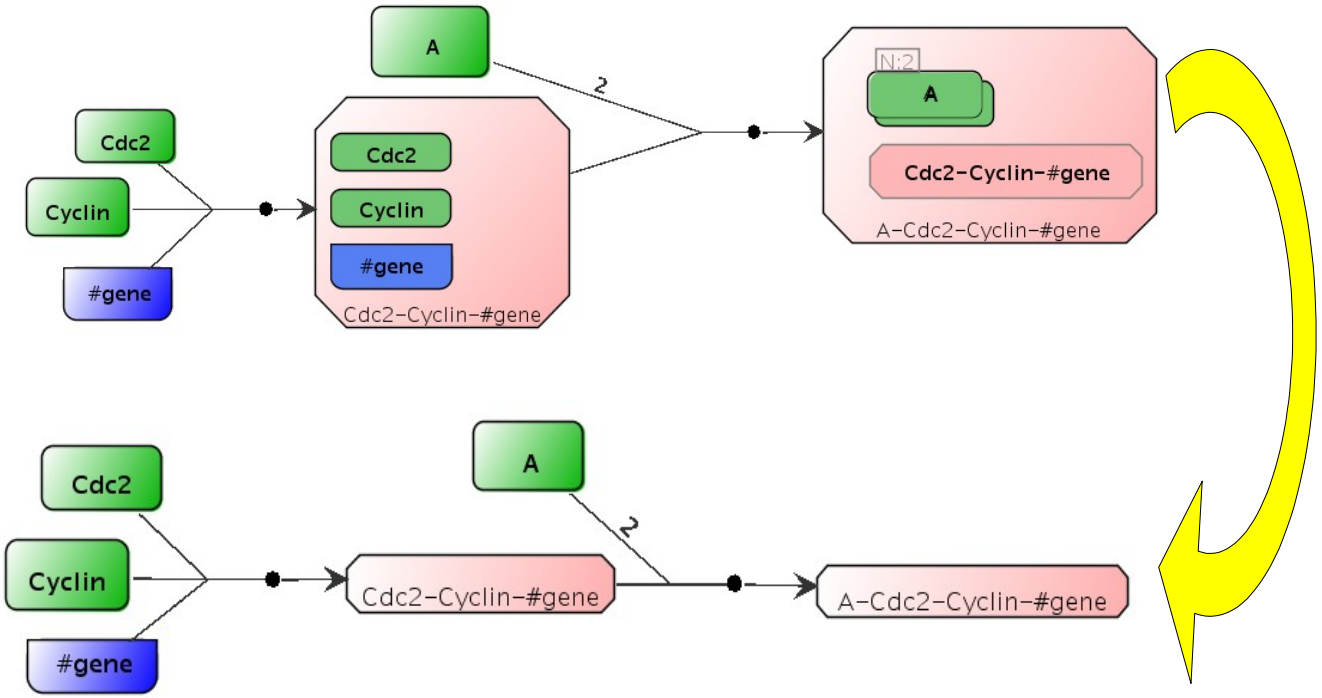
- *Nested complexes*



CONCLUSION

Proposal for SBGN

- *Nested complexes*



CONCLUSION

- *Biocham is based on a formal language for modelling biochemical systems*
- *Static analyses in the Graphical User Interface*
- *SBGN Graphical Editor - The best of the both worlds (formal and graphical)*

On-going work

- *Better automatic Layout*
- *Layout saving format and reuse of layout*
- *Generalization of graphical operations to edit model reductions [Gay Soliman Fages bioinformatics 2010]*

SBGN support in BIOCHAM

Thank You!!!!

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Thank You!!!!

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BIOCHAM