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

- [http://contraintes.inria.fr/biocham](http://contraintes.inria.fr/biocham)
- different simulators
- temporal logic based language
- features for correcting/completing/reducing/relating/coupling models

BIOCHAM MODEL Consists of

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

Modelling

Analysing

SBML compatible
**SBGN support in BIOCHAM**

**Analysing features in Biocham:**

- Simulations (Numerical, Boolean, Stochastic)
- Parameters Search
- Static analyses
  - parameters dimensions
  - kinetics consistency
  - influence graph
  - protein functions
  - model comparison
- Trace Analyse
- Model Checking
- Reduce Model
- Learn Rules – to complete or modify the model
- Revise Model using theory revision algorithm

**Biocham Model**
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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
  | molecule-(name,...,name) modified molecule
  | gene
  | ( molecule )

gene = #name
```

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 )

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**SBGN support in BioCham:**  

**SBGN Process Nodes and Arcs:**

**Process, Association and Dissociation; Consumption, Production and Modulation**

**Biocham reactions' grammar:**

\[
\text{reaction} = \begin{cases} \text{kine} & \text{tics for basic\_reaction} \\ | & \text{basic\_reaction} \\ | & \text{name : basic\_reaction} \\ | & \text{name : kine} & \text{tics for basic\_reaction} \end{cases}
\]

\[
\text{basic\_reaction} = \begin{cases} \text{solution} & \text{solution.} \\ | & \text{solution} & \text{solution} & \text{solution.} \\ | & \text{solution} & \text{solution} & \text{solution.} \\ | & \text{solution} & \text{solution} & \text{solution.} \end{cases}
\]

\[
\text{solution} = \begin{cases} & \text{_} | \text{object} | \text{integer\_object} | \text{solution} & \text{solution} | \text{solution} \end{cases}
\]
**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

- **Wrong kinetics**
  - Value of type `<reaction>` or `<set_of_reactions>` expected.

- **Wrong molecules name**
  - Two genes (≠ g1 and ≠ g2) are present in the left side of rule.
  - There are genes in left side of rule `a + #gene`, which are not in the right side.
  - Not enough parameters.
  - Too many parameters (or syntax error).
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]
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Thank You!!!!

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http://contraintes.inria.fr/BIOCHAM/
Thank You!!!!

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