Improved SBGN (ML) support in BioUML

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Motivation and aims

In BioUML mathematical model is represented as visual diagram. Each element of diagram may be associated with element (variable, equation) of mathematical model. BioUML provides several visual notations including Systems Biology Graphic Notation (SBGN PD) [2]. Diagram should be semantically correct according to both SBML and SBGN rules e.g. each reaction should have at least one reactant or product, each arc should be connected to appropriate glyph, etc. This is controlled automatically as user creates model. This process implies conversion process between SBML and SBGN and vice-versa and was implemented in BioUML earlier. However visual diagram created in BioUML could be easily passed to other tools only as SBML with layout and rendering information, moreover not every SBGN element was supported properly and several improvements were needed.

Results

Recently we have significantly improved support of SBGN and SBGN-ML in BioUML.

1. Logical operator is supported.
2. Phenotype is supported.
3. Ability set brush, pen and title font for each separate diagram element.
4. Creation of styles for similar customization of groups of elements.
5. Corrected visualization of process glyph.
6. BioUML-specific elements “subdiagram” and “port” replaced by SBGN “submap” and “tag”.
7. Automatic redraw of the diagram as user drags mouse.
8. SBGN-ML export and import including.
9. SBML objects are automatically parsed to correspondent SBGN classes (complex, macromolecule, simple chemical, association etc.) based on SBO term and annotation (hasParts).

Testing

For automatic nighlty testing we use reimport with check of models comparison.Another nighly test imports example SBGN-ML documents from www.sbgn.org] and generates report with comparison between diagrams from BioUML, other tools (VANTED [2], SBML Layout [3]) and figure from specification.

User may import SBGN-ML document, provide reaction rates, initial values and run simulation or export model as SBML. Thus we have implemented chain represented on fig. 1.

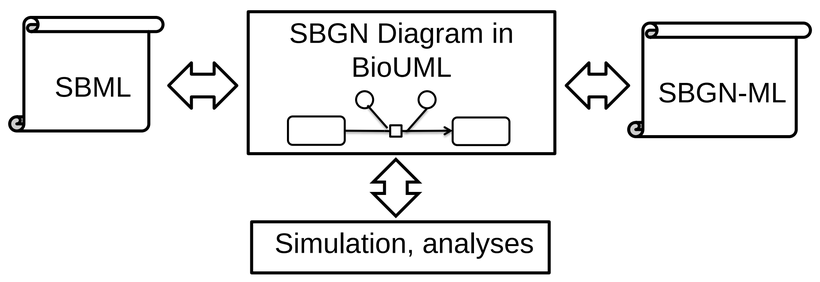

Fig.1. Relations between BioUML diagram, SBML and SBGN-ML

Discrepancies

There are few things that are not translated from SBML to SBGN (ML) or vice-versa.

1. Phenotype SBGN element has no mathematical meaning and is not translated to SBML.
2. SBML equations, events , functions and parameters are not represented in SBGN.

Availability

Described software is freely available as a part of open source platform BioUML at www.biouml.org

References

1. Moodie, Stuart, Le Novere, Nicolas , Demir, Emek, Mi, Huaiyu, and Villeger, Alice. Systems Biology Graphical Notation: Process Description language Level 1. Available from Nature Precedings <http://dx.doi.org/10.1038/npre.2011.3721.4> (2011).
2. Junker BH, Klukas C, Schreiber F.: VANTED: a system for advanced data analysis and visualization in the context of biological networks. *BMC Bioinformatics*. 2006;7(1):109. 10.1186/1471-2105-7-10.9
3. SBL Layout: http://sysbioapps.dyndns.org.

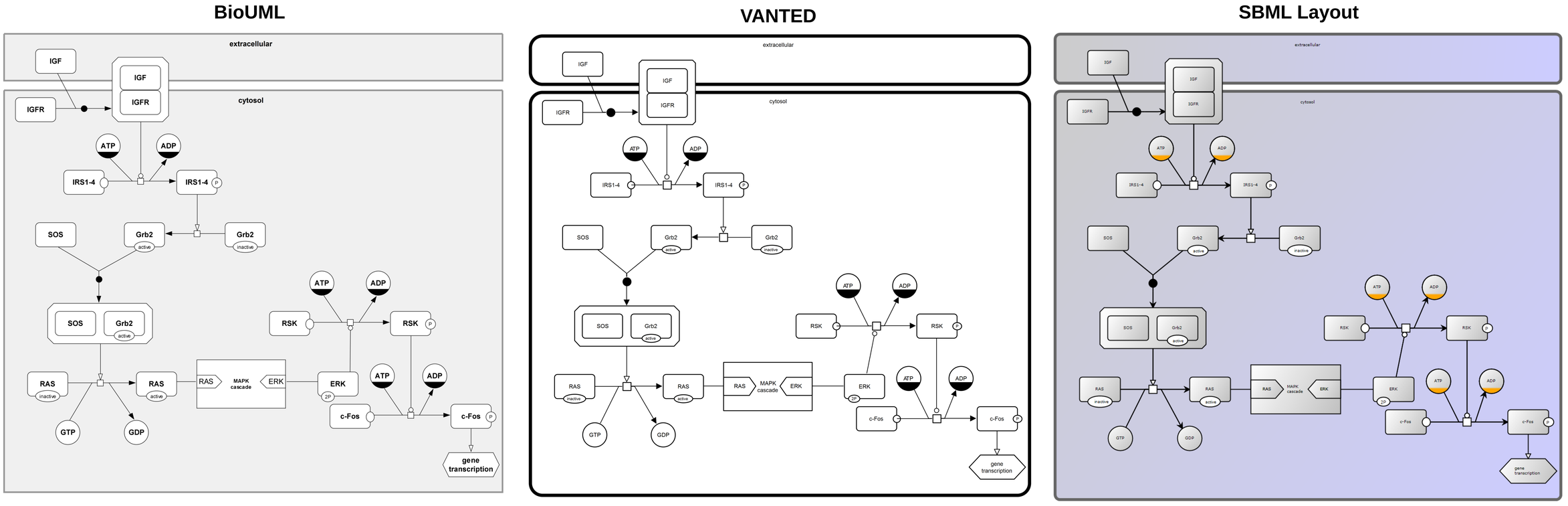

Fig. 2. Insulin signaling SBGN-ML document imported to three different tools: BioUML, VANTED, SBML Layout.

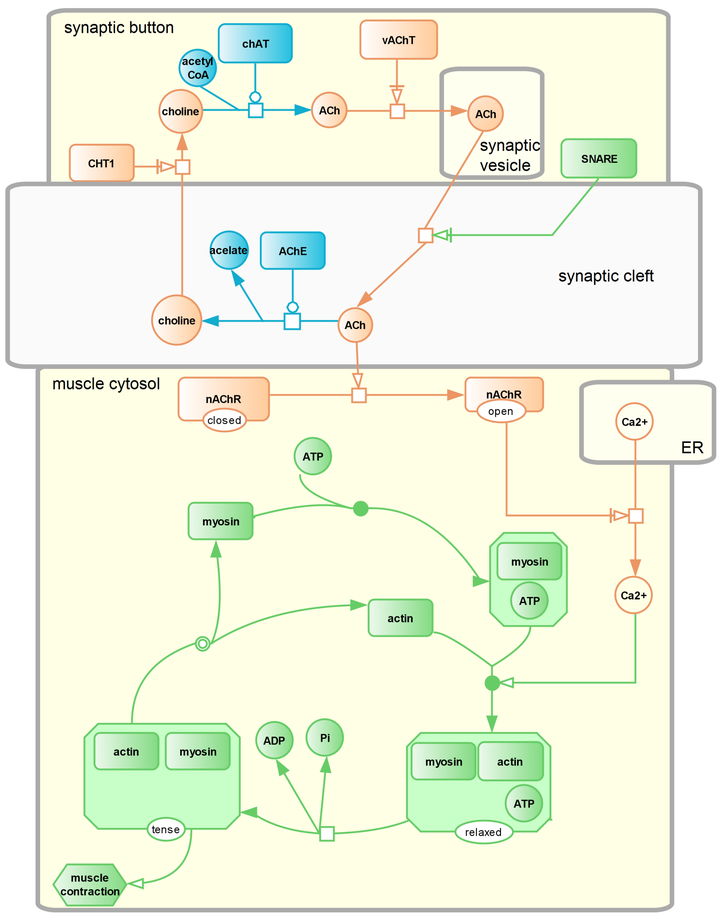

Fig. 3. Neuro-mascular junction SBGN diagram recreated in BioUML.

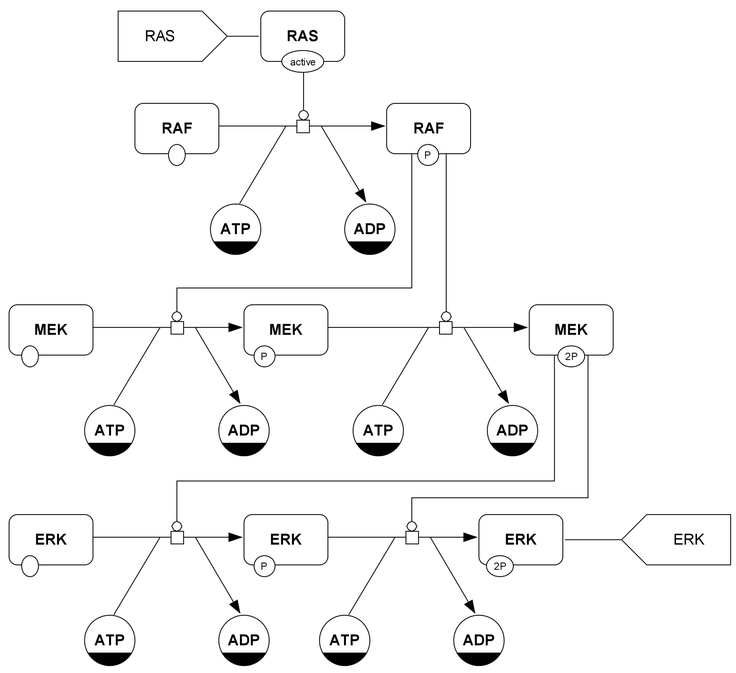

Fig. 4. MAPK cascade SBGN diagram recreated in BioUML.

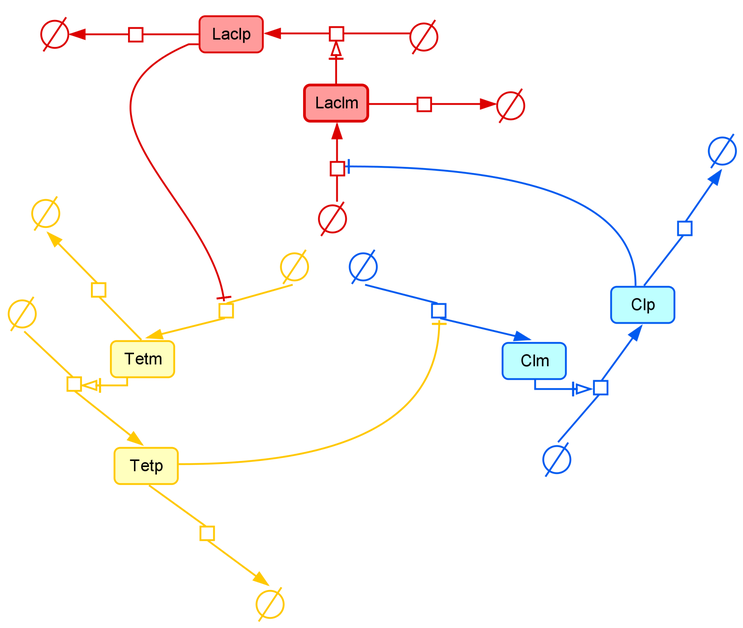

Fig. 5. Repressilator SBGN diagram recreated in BioUML.