Update on LibSBGN

Tobias Czauderna On behalf of the LibSBGN team

COMBINE 2012 17-08-2012

LibSBGN and SBGN-ML

- Community project started in 2009
 - facilitate development of SBGN supporting tools
 - increase interoperability between these tools
- Electronic implementation of SBGN
 - Exchange format for SBGN maps: SBGN-ML
 - XML schema based
 - express semantics, relationships and geometry
 - Software library to interact with SBGN maps: LibSBGN
 - object model and API
 - ▶ C++ and Java implementation
 - ▶ key features: reading, writing, validation, conversion and layout
- M.P. van Iersel, A.C. Villéger, T. Czauderna, S.E. Boyd,
 - F.T. Bergmann, A. Luna, E. Demir, A. Sorokin, U. Dogrusoz, Y. Matsuoka, A. Funahashi, M.I. Aladjem, H. Mi, S.L. Moodie, H. Kitano, N. Le Novère, F. Schreiber: **Software support for SBGN maps:**

SBGN-ML and LibSBGN. Bioinformatics, 28(15):2016-2021, 2012.

LibSBGN and SBGN-ML

- SourceForge project: http://libsbgn.sourceforge.net
 - ▶ Wiki: documentation, road map, "how to", useful links, ...
 - SVN repository: test suite, specs, XSD
- Mailing list: sbgn-libsbgn@lists.sourceforge.net
- Tools supporting SBGN-ML:
 - CellDesigner (Akira Funahashi)
 - Cytoscape SBGN plug-in (Martijn van Iersel)
 - PathVisio (Martijn van Iersel, Martina Kutmon)
 - Paxtools (Emek Demir)
 - SBGN-ED (Tobias Czauderna)
 - ▶ SBML Layout and Rendering Extension (Frank Bergmann)
 - VISIBIOweb (Ugur Dogrusoz)
- Databases supporting SBGN-ML:
 - ▶ Reactome (Robin Haw, David Croft)
 - MetaCrop (Falk Schreiber)
- Rendering comparison pipelinehttp://libsbgn.sourceforge.net/render_comparison/

LibSBGN and SBGN-ML

- Milestone 1 (released Januar 2011)
 - Support for Process Description language L1V1.2
 - ▶ Exchange shape, position, size
- Milestone 2 (released December 2011)
 - Support for Process Description language, Entity Relationship language, Activity Flow language
 - Validation based on Schematron
- Milestone 3 (planned for November 2012)
 - External references (SBML, BioPAX)
 - Complete support for submaps
 - Complete specification of any compartment shape
 - Support for color and line thickness
 - Update to latest version of each specification

94 </sbgn>

```
1 <sbgn xmlns="http://sbgn.org/libsbgn/0.2">
        <map language="process description">
                                                                                                                                                                      Extracellular space
          <notes>
          Glucose import followed by the first step of glycolysis.
          </notes>
          <qlyph compartmentRef="e" id="g" class="simple chemical">
                                                                                                                                                                                   Glucose
            <label text="Glucose"/>
            <br/>

          </glyph>
          <glyph compartmentRef="c" id="j" class="simple chemical">
            <label text="Glucose"/>
                                                                                                                                                                                                                   GLUT4
            <body><rr><box</r><br/><br/><br/><br/>y="155" x="55" h="30" w="30"/>
         </glyph>
         <glyph id="f" class="process">
            <body><box y="112" x="62" h="16" w="16"/>
           <port y="138" x="70" id="r"/>
            <port y="102" x="70" id="s"/>
         </qlyph>
          <glyph compartmentRef="c" id="k" class="simple chemical">
            <label text="ATP"/>
21
            <clone/>
            <body><box y="175" x="15" h="30" w="30"/>
22
          </qlyph>
          <glyph compartmentRef="c" id="m" class="macromolecule">
            <label text="Hexokinase"/>
                                                                                                                                                                                  Glucose
            <body><box y="185" x="85" h="30" w="70"/>
            <glyph id="n" class="state variable">
27
                                                                                                                                                                                                               active
                                                                                                                                                          ATP
            <label text="active"/>
            <body><br/><box<br/>y="179" x="96" h="12" w="30"/></br>
                                                                                                                                                                                                          Hexokinase
            </glyph>
30
31
         </glyph>
          <glyph compartmentOrder="2" id="e" class="compartment">
            <label text="Extracellular space"/>
            <br/>
<box>
y="5" x="5" h="70" w="160"/>
          </glyph>
         <arc target="s" source="g" id="a" class="consumption">
            <start y="55" x="70"/>
81
            <end y="102" x="70"/>
82
83
          </arc>
                                                                                                                                                         ADP
          <arc target="j" source="r" id="u" class="production">
            <start y="138" x="70"/>
85
            <end y="155" x="70"/>
86
          </arc>
         <arc target="f" source="h" id="v" class="catalysis">
                                                                                                                                                                                     G<sub>6</sub>P
           <start y="95" x="120"/>
            <next y="120" x="120"/>
            <end y="120" x="78"/>
         </arc>
                                                                                                                                                                                          Cytosol
93 </map>
```

1

2

3

4

5

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93 </map>
94 </sbgn>
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```
1 <sbqn xmlns="http://sbqn.org/libsbqn/0.2">
                                          <map language="process description">
                                                                                                                                                                                       Extracellular space
                                            <notes>
                     <qlyph id="f" class="process">
14
                         <bbox y="112" x="62" h="16" w="16"/>
15
                         <port y="138" x="70" id="r"/>
16
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17
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18
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                                             </glyph>
                     <glyph compartmentRef="c" id="k" class="simple chemical">
19
                     <label text="ATP"/>
20
21
                     <clone/>
22
                         <bbox y="175" x="15" h="30" w="30"/>
                     </glyph>
23
                                                <Start y= 130 X= /0 /
                                              <end y="155" x="70"/>
                                            </arc>
                                            <arc target="f" source="h" id="v" class="catalysis">
                                                                                                                                                                                                      G<sub>6</sub>P
                                             <start y="95" x="120"/>
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                                              <clone/>
                                              <bbox y="175" x="15" h="30" w="30"/>
                                           </glyph>
                     <arc target="j" source="r" id="u" class="production">
84
                         <start y="138" x="70"/>
85
                         <end y="155" x="70"/>
86
87
                    </arc>
                    <arc target="f" source="h" id="v" class="catalysis">
88
                         <start y="95" x="120"/>
89
                         <next y="120" x="120"/>
90
                         <end y="120" x="78"/>
91
92
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                                           <arc target="f" source="h" id="v" class="catalysis">
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                                            </arc>
                                                                                                                                                                                                         Cytosol
                                    93 </map>
```

Java example (available from http://libsbgn.sourceforge.net)

```
// our sbgnml file goes in "f"
File f = new File ("../test-files/adh.sbgn");
// Now read from "f" and put the result in "sbgn"
Sbgn sbgn = SbgnUtil.readFromFile(f);
// map is a container for the glyphs and arcs
Map map = sbqn.qetMap();
// we can get a list of glyphs (nodes) in this map with getGlyph()
for (Glyph q : map.qetGlyph())
    // print the sbgn class of this glyph
    System.out.print (" Glyph with class " + q.getId());
    // if there is a label, print it as well
    if (q.getLabel() != null)
        System.out.println (", and label " + g.getLabel().getText());
    else
        System.out.println (", without label");
// we can get a list of arcs (edges) in this map with getArc()
for (Arc a : map.getArc())
    // print the class of this arc
    System.out.println (" Arc with class " + a.getClazz());
```

LibSBGN Community

Mirit Aladjem (MIM)

Frank Bergmann (SBML Layout)

Sarah Boyd (Dunnart)

Tobias Czauderna (SBGN-ED)

Emek Demir (Paxtools)

Ugur Dogrusoz (VISIBIOweb)

Akira Funahashi (CellDesigner)

Hiroaki Kitano (CellDesigner)

Nicolas Le Novère (BioModels Database)

Augustin Luna (MIM)

Yukiko Matsuoka (CellDesigner)

Huaiyu Mi (PANTHER Pathways)

Stuart Moodie (EPE)

Falk Schreiber (SBGN-ED)

Anatoly Sorokin (EPE)

Martijn van Iersel (PathVisio)

Alice Villéger (Arcadia)

http://libsbgn.sourceforge.net