LibSBGN Current Status and Future Plans

Tobias Czauderna, Martijn van Iersel COMBINE 2011, Heidelberg

Background Context & Motivation

WHY LIBSBGN?

Many tools support SBGN

- Arcadia
- Athena
- BiNoM
- BioModels Database
- BioPAX
- BioUML
- ByoDyn
- CellDesigner
- Dunnart
- Edinburgh Pathway Editor

- JWS Online
- Mayday
- Netbuilder (Apostrophe)
- PANTHER
- PathVisio
- PathwayLab
- Reactome
- Vanted
- VISIBIOweb
- ... 19 tools (and still counting)

See http://sbgn.org/SBGN Software

The problem with SBGN tools

- No interchange of maps
- No reuse of code
 - Useful features (e.g. validation, layout) are scattered across tools, and code is duplicated.

Solution? LibSBGN

- Goals
 - Improve Interoperability
 - Encourage code re-use
 - Help development of SBGN compliant tools

Solution? LibSBGN

LibSBGN consists of 2 parts

- Exchange format: SBGN-ML
 - XML Schema based
 - express semantics, relationships and geometry
- Software library: LibSBGN
 - Java and C++
 - key features: reading, writing, validation, conversion and layout

Why SBGN-ML?

PNG / SVG

you lose biological network

BioPAX

you lose the layout

GML / GraphML

not standard

SBML-Layout

you lose SBGN semantics

Development Methods & Infrastructure

HOW IT'S DONE

Community project

- Mirit Aladjem (MIM)
- Frank Bergmann (SBML Layout)
- Michael Blinov (BioNetGen)
- Sarah Boyd (Dunnart)
- Tobias Czauderna (VANTED)
- Emek Demir (Pathway Commons)
- Ugur Dogrusoz (Patika)
- Akira Funahashi (CellDesigner)
- Hiroaki Kitano (CellDesigner)

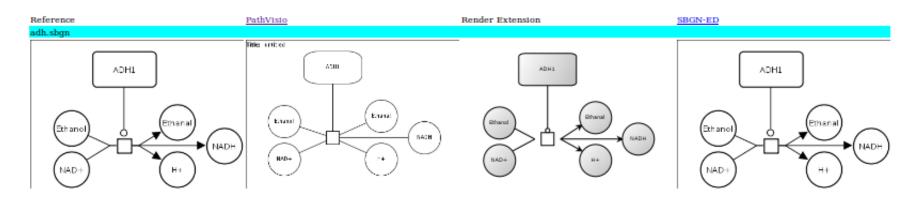
- Nicolas Le Novère (BioModels Database)
- Augustin Luna (MIM)
- Yukiko Matsuoka (CellDesigner)
- Huaiyu Mi (PANTHER Pathway)
- Stuart Moodie (EPE)
- Falk Schreiber (VANTED)
- Anatoly Sorokin (EPE)
- Martijn van Iersel (PathVisio)
- Martina Kutmon (PathVisio)
- Alice Villéger (Arcadia)
- Gael Jalowicki (Biomodels)

Organization

- Mailing list: <u>sbgn-libsbgn@lists.sourceforge.net</u>
- Monthly online meetings
 - minutes and announcement on mailing list
 - on EVO: http://evo.caltech.edu
- SourceForge project: http://libsbgn.sourceforge.net
 - Wiki: documentation, road map, "how to", useful links, ...
 - Tracker: "to do" list (bugs and missing features)
 - SVN repository: test suite, specs, XSD, validation rules
- Quality control
 - Rendering comparison pipeline http://libsbgn.sourceforge.net/rendering comparison

Development infrastructure

- **Test suite**: test cases (so far):
 - 25 for PD
 - 17 for ER
 - 8 for AF
 - SBGN map in PNG format
 - corresponding SBGN-ML file
- Rendering comparison pipeline



Current Status

WHERE WE ARE

SBGN-ML Roadmap

Milestone 1 released (Jan. 2011)

- Only support for SBGN PD
- Only high-level graphics specification
- Basic validation using XML Schema

Milestone 2 (planned for Oct. 2011)

- Implement semantics for all 3 languages:
 SBGN PD, ER and AF
- Extra validation using Schematron
- Third-party extensibility

Milestone 3

- Complete graphical specification
- Submaps...

Milestone 4

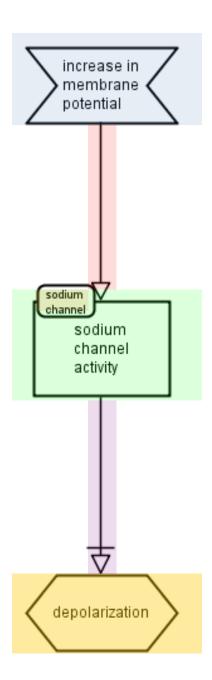
Linking, MIRIAM compatibility, ...

What is new (since Harmony)

- More test cases
- Schematron rulesets
- Third-party extensibility
- AF support
- compartmentRef and compartmentOrder
- Id's for Arcs are compulsory
- Arcgroups

Brief SBGN-ML overview

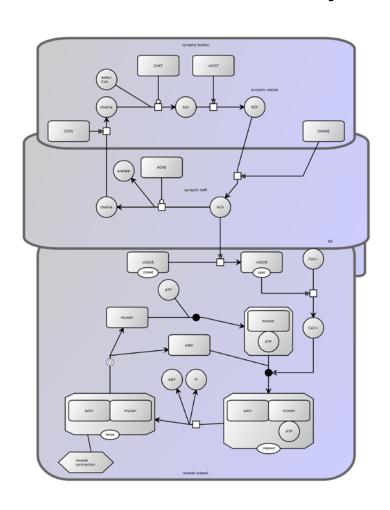
- Main requirements
 - Easy to draw (explicit coordinates)
 - Easy to interpret (network and semantics)
- Top level: Map element
- Most important elements: Glyph and Arc
 - "class" attribute determines semantics, e.g.
 "macromolecule"
- Glyph geometry: bounding box only
- Arcs refer to glyph or glyph ports (network connectivity)

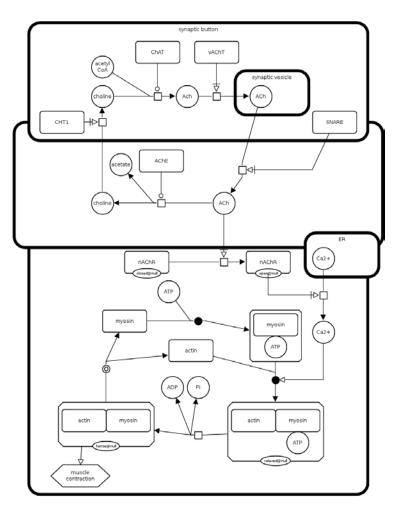


```
<?xml version="1.0" encoding="UTF-8"?>
 2
     -<sbgn xmlns="http://sbgn.org/libsbgn/0.2">
 3
           <map language="activity flow">
 4
 5
               <qlyph class="perturbation" id="q1">
                   <label text="increase in&#xA;membrane&#xA;potential"/>
 6
 7
                   <bbox x="30" y="30" w="120" h="60"/>
8
               </glyph>
9
10
               <qlyph class="biological activity" id="g2">
11
                   <label text="sodium&#xA; channel&#xA; activity"/>
12
                   <bbox x="36" y="232" w="108" h="75"/>
13
                   <qlyph class="unit of information" id="q2.1">
14
                       <label text="sodium&#xA; channel"/>
                       <entity name="macromolecule"/>
15
                       <bbox x="39" y="219" w="46" h="26"/>
16
                   </qlyph>
17
               </qlyph>
18
19
20
               <qlyph class="phenotype" id="q3">
21
                   <label text="depolarization"/>
22
                   <bbox x="30" y="450" w="120" h="60"/>
23
               </glyph>
24
25
               <arc class="positive influence" source="q1" target="q2" id="a1">
26
                   <start x="90" y="90" />
27
                   <end x="90" v="232" />
28
               </arc>
29
               <arc class="necessary stimulation" source="g2" target="g3" id="a2">
30
31
                   <start x="90" y="307" />
32
                   <end x="90" y="450" />
33
               </arc>
34
35
           </map>
      </sbgn>
36
```

```
increase in
                             <?xml version="1.0" encoding="UTF-8"?>
 membrane
                            -<sbqn xmlns="http://sbqn.org/libsbqn/0.2">
 potential
                                <map language="activity flow">
                                   <qlyph class="perturbation" id="q1">
                                       <label text="increase in&#xA; membrane&#xA; potential"/>
                                       <bbox x="30" y="30" w="120" h="60"/>
                                    </alvoh>
                <glyph class="biological activity" id="g2">
                      <label text="sodium&#xA;channel&#xA;activity"/>
                      <bbox x="36" y="232" w="108" h="75"/>
                      <glyph class="unit of information" id="g2.1">
sodium
channel
                            <label text="sodium&#xA;channel"/>
   sodium
   channel
                            <entity name="macromolecule"/>
   activity
                            <bbox x="39" y="219" w="46" h="26"/>
                     </glyph>
                </glyph>
                                       <end x="90" y="232" />
                        28
                                   </arc>
                        29
                                   <arc class="necessary stimulation" source="q2" target="q3" id="a2">
                        30
                                       <start x="90" y="307" />
                        31
                                      <end x="90" v="450" />
                        32
                        33
                                    </arc>
                        34
                        35
                                </map>
                        36
                             </sbgn>
depolarization
```

compartmentOrder & compartmentRef





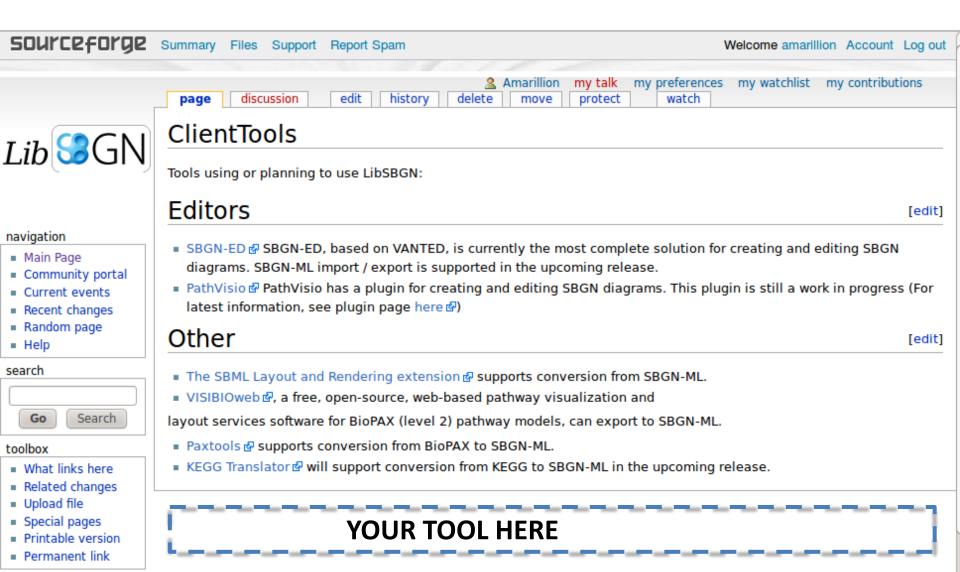
Extensions

```
<map language="process description">
   <extension>
       <renderInformation id="example" programName="SBML Layout"</pre>
           programVersion="3.0"
           xmlns="http://projects.eml.org/bcb/sbml/render/level2">
           <colorDefinition id="yelloComp" value="#ffffccff" />
           </listOfColorDefinitions>
       </renderInformation>
   </extension>
```

Future Plans

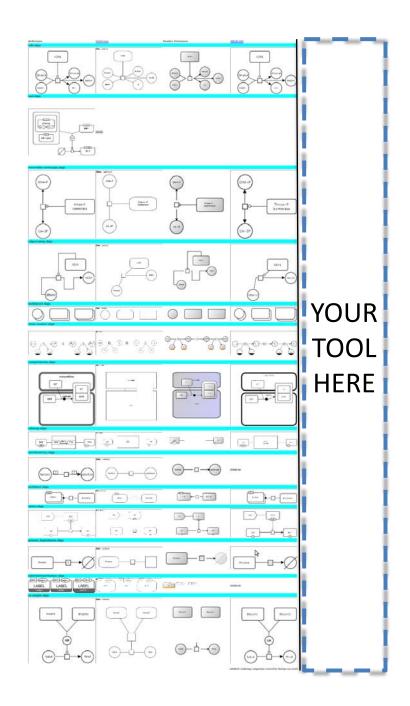
WHAT NEXT?

Software support



Software support

- Conversion SBGN-ML -> PNG
 - PathVisio (Martijn van Iersel)
 - 2. SBGN-ED (Tobias Czauderna)
 - 3. SBML Layout (Frank Bergmann)



What's next

- Release (Soon October 2011)
- More detailed graphics
 - Roundness of rounded rectangles
 - Arrow-glyph size
 - Line thickness
 - **—** ...
- Better handling of submaps

THANK YOU

- To everyone involved so far: GOOD JOB TEAM
- To all developers supporting SBGN (or planning to):
 feel free to join the club!
 - Use the library and support the schema
 - Take part in online discussions
 - Contribute content to the SourceForge project

http://libsbgn.sourceforge.net