### Introduction to LibSBGN

# Tobias Czauderna IPK Gatersleben, Germany

HARMONY 2012 21-05-2012

#### SBGN

- "...an effort to standardize the graphical notation used in maps of biochemical and cellular processes studied in systems biology."
- Exchange of knowledge
- Can graphically represent quantitative models, biochemical pathways, transcriptional regulatory networks and more, at different levels of granularity
- Developed over years by a growing community (since 2006)
- Three languages

▶ Process Description → one state = one glyph

▶ Entity Relationship → one entity = one glyph

▶ Activity Flow → conceptual level

http://sbgn.org

#### 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

#### 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)
- Rendering comparison pipelinehttp://libsbgn.sourceforge.net/render\_comparison/

#### LibSBGN and SBGN-ML

- Milestone 1
  - Support for Process Description language
  - ▶ Exchange shape, position, size
- Milestone 2 December 2011
  - Support for Entity Relationship language, Activity Flow language
  - Validation

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<br/><br/><br/><br/>y="155" x="55" h="30" w="30"/></rr>
         </glyph>
         <glyph id="f" class="process">
            <body><br/><body><br/><br/><br/><br/>y="112" x="62" h="16" w="16"/></br>
           <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

```
<sbgn xmlns="http://sbgn.org/libsbgn/0.2">
  <map language="process description">
    <notes>
    Glucose import followed by the first step of glycolysis.
  </notes>
```

```
<glyph id="f" class="process">
             <body><box y="112" x="62" h="16" w="16"/>
           <port y="138" x="70" id="r"/>
           <port v="102" x="70" id="s"/>
          </qlyph>
           <glyph compartmentRef="c" id="k" class="simple chemical">
             <label text="ATP"/>
             <clone/>
              <br/>
<box v="175" x="15" h="30" w="30"/>
           </qlyph>
           <glyph compartmentRef="c" id="m" class="macromolecule">
              <label text="Hexokinase"/>
                                                                                                                                                                                                                                Glucose
              <br/>
bbox v="185" x="85" h="30" w="70"/>
             <glyph id="n" class="state variable">
                                                                                                                                                                                                                                                                    active
                                                                                                                                                                                                 ATP
             <label text="active"/>
             <br/>

                                                                                                                                                                                                                                                              Hexokinase
             </qlyph>
          </qlyph>
           <qlyph compartmentOrder="2" id="e" class="compartment">
             <label text="Extracellular space"/>
              <br/>
<box>
y="5" x="5" h="70" w="160"/>
           </qlyph>
          <arc target="s" source="g" id="a" class="consumption">
              <start y="55" x="70"/>
              <end y="102" x="70"/>
82
           </arc>
83
                                                                                                                                                                                                ADP
           <arc target="j" source="r" id="u" class="production">
             <start y="138" x="70"/>
             <end y="155" x="70"/>
86
           </arc>
          <arc target="f" source="h" id="v" class="catalysis">
                                                                                                                                                                                                                                    G6P
            <start y="95" x="120"/>
             <next y="120" x="120"/>
              <end y="120" x="78"/>
          </arc>
                                                                                                                                                                                                                                         Cytosol
93 </map>
94 </sbgn>
```

```
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
                         <port y="102" x="70" id="s"/>
17
                   </glyph>
18
                                             <port y="102" x="70" id="s"/>
                                            </qlyph>
                                             <glyph compartmentRef="c" id="k" class="simple chemical">
                                              <label text="ATP"/>
                                              <clone/>
                                               <br/>
<box v="175" x="15" h="30" w="30"/>
                                             </qlyph>
                                             <glyph compartmentRef="c" id="m" class="macromolecule">
                                               <label text="Hexokinase"/>
                                                                                                                                                                                                   Glucose
                                               <br/>

                                              <glyph id="n" class="state variable">
                                                                                                                                                                                                                             active
                                                                                                                                                                             ATP
                                              <label text="active"/>
                                              <body><br/><box<br/>y="179" x="96" h="12" w="30"/></br>
                                                                                                                                                                                                                        Hexokinase
                                             </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"/>
                                              <next y="120" x="120"/>
                                              <end y="120" x="78"/>
                                            </arc>
                                                                                                                                                                                                          Cytosol
                                     93 </map>
                                     94 </sbgn>
```

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><br/><br/><br/><br/>y="155" x="55" h="30" w="30"/></br/>
                                            </glyph>
                                            <glyph id="f" class="process">
                                              <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"/>
                                              <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
                     </arc>
                                           <arc target="f" source="h" id="v" class="catalysis">
                                                                                                                                                                                                    G6P
                                            <start y="95" x="120"/>
                                            <next y="120" x="120"/>
                                             <end y="120" x="78"/>
                                            </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