

# LibSBGN

## Current Status and Future Plans

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Background Context & Motivation

# **WHY LIBSBGN?**

# Growing SBGN software support

- Arcadia
  - Athena
  - BiNoM
  - BioModels Database
  - BioPAX
  - BioUML
  - ByoDyn
  - CellDesigner
  - Dunnart
  - Edinburgh Pathway Editor
  - JWS Online
  - Mayday
  - Netbuilder (Apostrophe)
  - PANTHER
  - PathwayLab
  - Reactome
  - Vanted
  - VISIBIOweb
  - ... 19 tools (and still counting)
- Cf. [http://sbgn.org/SBGN\\_Software](http://sbgn.org/SBGN_Software)

# Multiple electronic representations

- **Model** (= network + biological semantics ) + **layout + rendering**
  - SBML + layout and rendering extension
  - Celldesigner SBML
  - BioPAX + layout extension
  - CellML + layout information?
- **Graph + layout + rendering**
  - GraphML + yFiles extension
  - GML
- **Images**
  - vector (e.g. SVG, PDF)
  - bitmap (e.g. PNG, TIFF)
- Custom-made formats...

# Lack of interoperability

- **Users can't transfer maps** between tools
  - But features they need (e.g. validation, layout) may be scattered across different pieces of software!
- **Developers can't reuse** each others' code
  - The same set of core features (e.g. conversion to and from usual formats) gets implemented multiple times...

# Solution? LibSBGN

- **Community project** started at SBGN 4.5 in 2009
  - facilitate development of SBGN compliant tools
  - increase interoperability between these tools
- Electronic implementation of SBGN
  - **Exchange format** for all SBGN maps: **SBGN-ML**
    - XML based
    - express semantics, relationships and geometry
  - **Software library** to interact with SBGN maps: **LibSBGN**
    - object model and API, in Java and C++
    - key features: conversion, validation and layout

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)
- **Alice Villéger** (Arcadia)

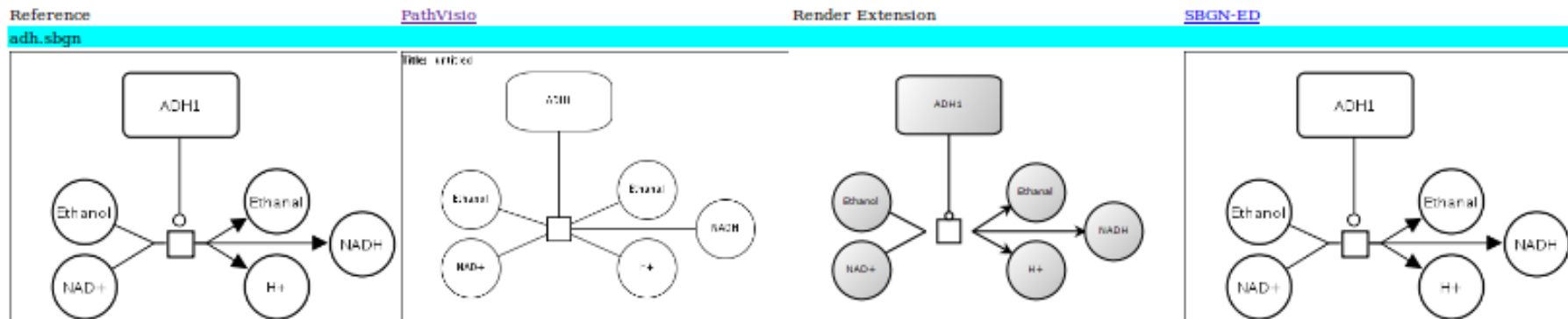


# Online workspace

- **Mailing list:** [sbgn-libsbn@lists.sourceforge.net](mailto:sbgn-libsbn@lists.sourceforge.net)
- **Monthly online meetings**
  - first on Skype, now on **EVO**: <http://evo.caltech.edu>
  - **minutes** and **announcement** on mailing list
  - **scheduled** on Doodle: <http://www.doodle.com/>
  - **agenda** on wiki
- SourceForge project: <http://libsbn.sourceforge.net>
  - **Wiki**: documentation, road map, “how to”, useful links, ...
  - **Tracker**: “to do” list (bugs and missing features)
  - **SVN** repository: test suite, specs, XSD
- “Quality control” tools
  - **Automatic XSD validation** against examples on test server  
<http://azraelbigcat.dyndns.org/reports/libsbn/>
  - **Rendering comparison** pipeline  
[http://www.bigcat.unimaas.nl/~martijn/render\\_comparison](http://www.bigcat.unimaas.nl/~martijn/render_comparison)

# Core development infrastructure

- **Test suite:** 15 test cases (so far)
  - SBGN diagram (PNG)
  - corresponding SBGN-ML file
- Rendering comparison pipeline



# Typical workflow?

- 1 Someone notices a **problem in the SVN repository**
  - e.g. bug or missing feature
- 2 Notify the community
  - file a **bug report** in the tracker
  - send a message to the **mailing list**
- 3 Discussions
  - monthly online meetings: periodic **tracker review**
  - mailing list: **review** all **major decisions**
- 4 Resolution
  - **commit new version** in SVN repository
  - **close issue** in tracker

Current Status

**WHERE WE ARE**


# SBGN-ML Roadmap (cf. wiki)

- **Milestone 1**
  - Implement semantics of SBGN PD L1v1.1
  - Only high-level graphics specification
  - XML Schema available for validation
- **Milestone 2**
  - Implement semantics for all 3 languages: SBGN PD, ER and AF
- **Milestone 3**
  - Support for detailed graphics specification

# SBGN-ML Roadmap (cf. wiki)

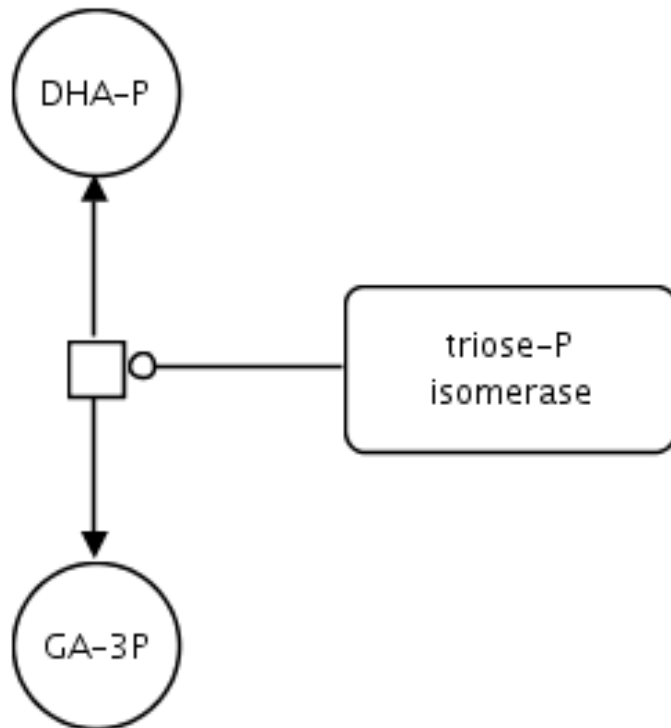
- **Milestone 1** ← *we're about there...*
  - Implement semantics of SBGN PD L1v1.1
  - Only high-level graphics specification
  - XML Schema available for validation
- **Milestone 2**
  - Implement semantics for all 3 languages: SBGN PD, ER and AF
- **Milestone 3**
  - Support for detailed graphics specification

# Brief SBGN-ML overview

- Main requirements
  - **Easy to draw** (explicit coordinates)
  - **Easy to interpret** (network and semantics)

Somewhat redundant,  
but that's a choice
- Only two top-level elements: **Glyph** and **Arc**
  - “class” attribute determines semantic → rendering
- Glyph geometry: **bounding box** only
- Glyph children:
  - label
  - other glyphs (e.g. state variable, unit of information)
  - ports where arcs can connect
- Arcs **refer to glyph** or glyph ports (network connectivity)
- Arcs contain an **optional route** (list of lines and Bezier curves)

# Example



```
<?xml version="1.0" encoding="UTF-8"?>
<sbgn xmlns="http://sbgn.org/libsbgn/pd/0.1">

  <glyph class="simple chemical" id="glyph1">
    <label text="DHA-P"/>
    <bbox x="30" y="20" w="60" h="60"/>
  </glyph>
  <glyph class="simple chemical" id="glyph2">
    <label text="GA-3P" />
    <bbox x="30" y="220" w="60" h="60"/>
  </glyph>
  <glyph class="macromolecule" id="glyph3">
    <label text="Triose-P&#xA;Isomerase" /> <!-- contains line break -->
    <bbox x="150" y="120" w="120" h="60"/>
  </glyph>

  <glyph class="process" orientation="vertical" id="pn1">
    <bbox x="50" y="140" w="20" h="20"/>
    <port x="60" y="130" id="pn1.1"/>
    <port x="60" y="170" id="pn1.2"/>
  </glyph>

  <arc class="production">
    <source x="60" y="130" ref="pn1.1" />
    <target x="60" y="80" ref="glyph1" />
  </arc>

  <arc class="production">
    <source x="60" y="170" ref="pn1.2" />
    <target x="60" y="220" ref="glyph2" />
  </arc>

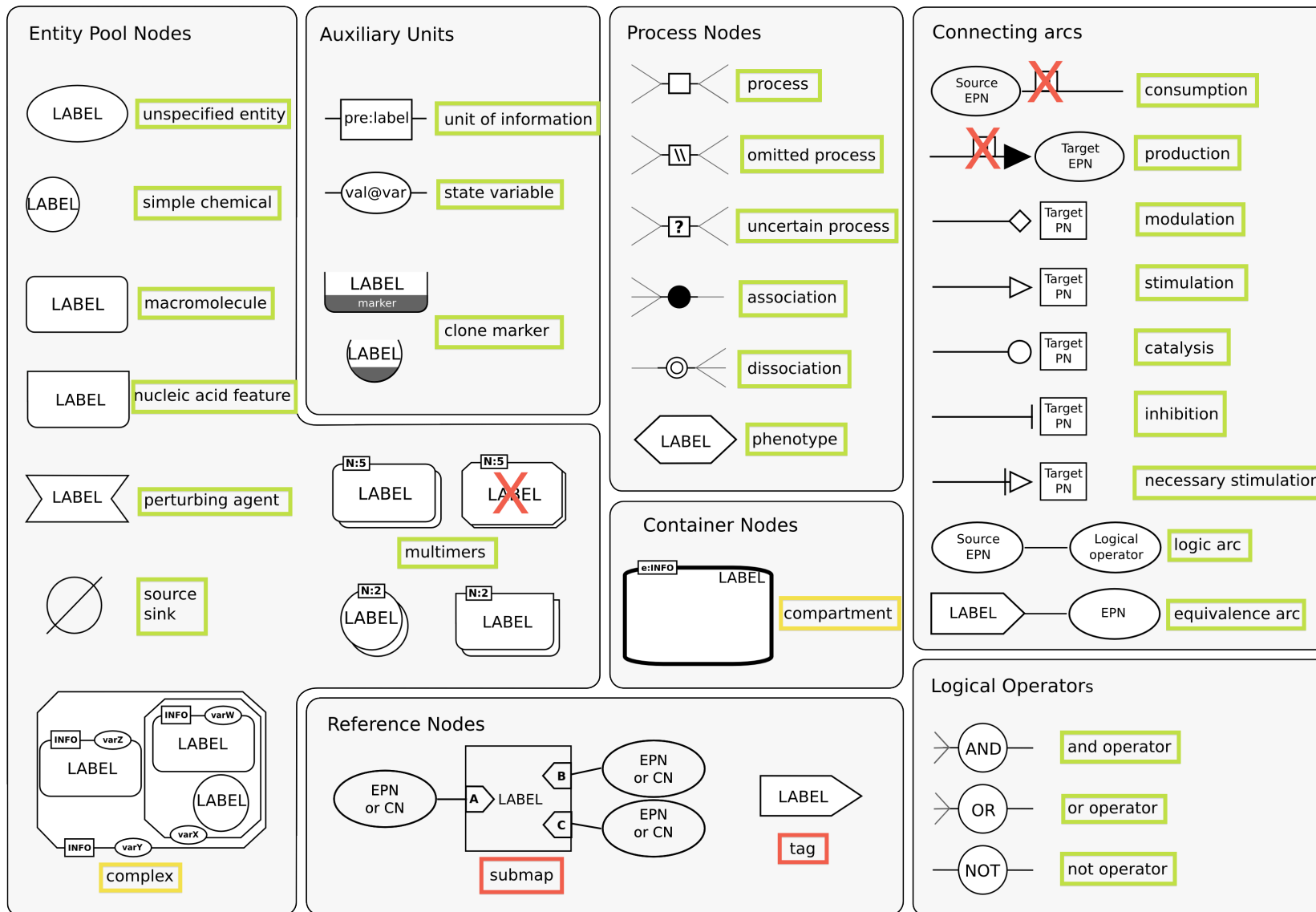
  <arc class="catalysis">
    <source x="150" y="150" ref="glyph3" />
    <target x="70" y="150" ref="pn1" />
  </arc>

</sbgn>
```



# SBGN-ML v1

- Current status
  - supports **almost all SBGN-PD semantics**
  - describes **network connectivity**
  - stores **essential layout information**
- Pending issues
  - describing **arc routes** (almost ready)
  - discuss **containment**: at COMBINE?
    - complex, compartments, submaps?
- **Ready for developer adoption**



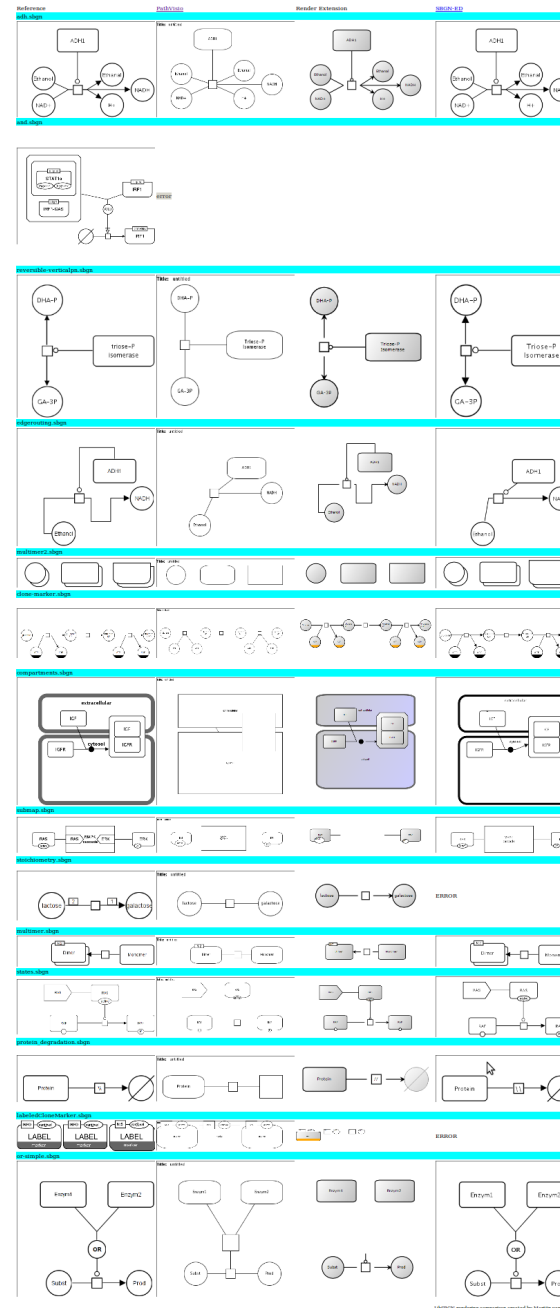
Stable

Needs some work

Currently missing

# Software support

- LibSBGN prototype:  
**SBGN-ML parser**
    - automatic Java binding with JAXB
  - 3 compatible tools
    - PathVisio (Martijn van Iersel)
    - SBGN-ED (Tobias Czauderna)
    - SBML Layout (Frank Bergmann)
- ➔ featured in the **rendering comparison gallery**



YOUR  
TOOL  
HERE

Future Plans

**WHAT NEXT?**

# Short to mid-term plans

- During COMBINE
  - break-out sessions at any time: meet at LibSBGN poster?
  - **monthly technical meeting on Thursday at lunch time**
  - “governance” discussions on last day?
- SBGN-ML
  - **release version 1?** (pretty soon, but only when it’s ready)
  - support for other SBGN languages (Milestone 2)
- LibSBGN
  - C++ parser <http://www.codesynthesis.com/products/xsd/>
  - complete **validation**
  - **conversion** to and from SBML and BioPAX

# 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**
    - Your tool could feature in the render comparison gallery
  - Take part in online discussions
    - Make your **requirements** heard!
  - **Contribute content** to the SourceForge project
    - Just ask any of the project members to get added

<http://libsbgn.sourceforge.net>