

Arcadia

A visualisation software
for metabolic pathways

Alice Villéger

alice.villeger@manchester.ac.uk

Bioanalytical Sciences Group
School of Chemistry, Faculty of EPS

University of Manchester

www.manchester.ac.uk

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Outline

- Project background
 - specifications
- Current implementation
 - short demo
- Future plans
 - SBGN support

Context

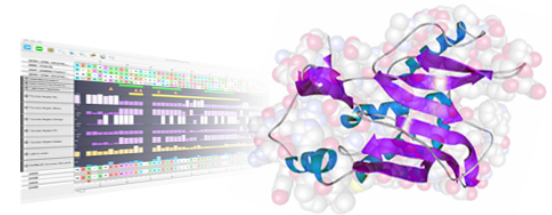
- Project(s)
 - Initiated/coordinated by Prof. Douglas Kell
 - Head of the Bioanalytical Sciences Group
 - Location: Manchester **Interdisciplinary** Biocentre
 - Collaboration between people from \neq backgrounds
 - biochemists, system biologists, computer scientists, ...
- Cornerstone
 - visualisation software for metabolic pathways

Design considerations

- Viewer ≠ Editor
 - Simple interface
 - Multiple views (= different perspectives)
 - Focus on navigation
- Light-weight stand-alone component
 - VS full integrated environment “swiss army knife” approach
 - Easy to deploy and maintain
 - Interoperable ⇒ support existing standards

Reference: Utopia framework

- Collection of desktop tools for protein analysis
 - molecule viewer, sequence alignment tool, etc.
- Characteristics
 - Seamless integration of heterogeneous resources
 - local files, local tools, remote databases, web services
 - Intuitive and flexible visualisation interface
 - Semantically rich data model
 - supports many \neq annotation types



Implementation

Arcadia = extension of Utopia

- C++ \Rightarrow object-oriented programming
 - Model/View/Controller architecture
- Cross-platform
 - Windows, MacOS, Unix/Linux support
- Open source
 - SVN repository (when released)

Implementation ++

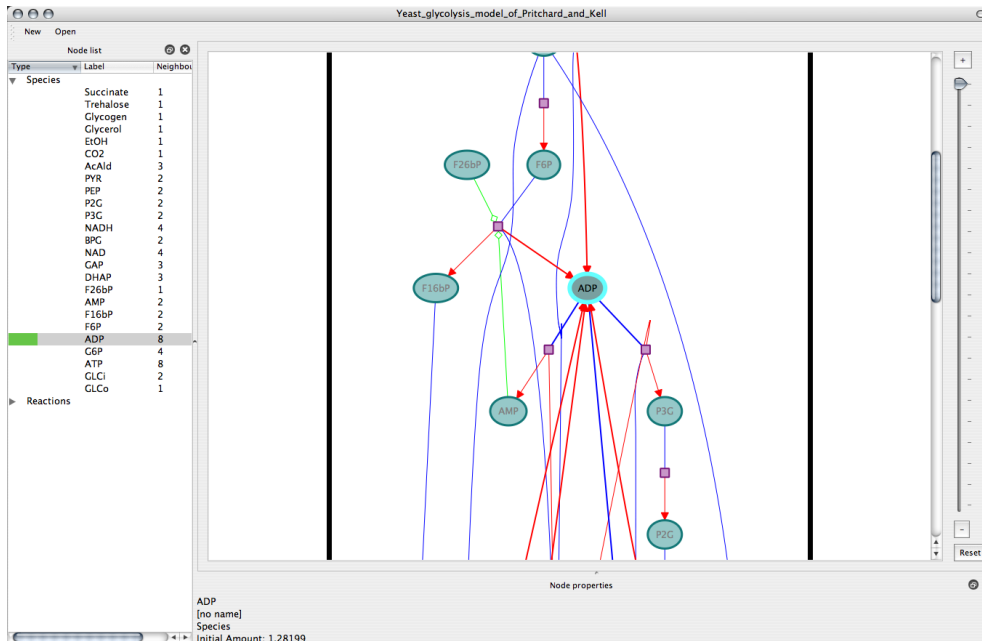
Built on top of powerful existing libraries:

- LibSBML \Rightarrow SBML support
- Boost Graph Library \Rightarrow generic graph model
- Qt (Trolltech) \Rightarrow GUI
- GraphViz \Rightarrow node layout algorithms
- LibAvoid \Rightarrow edge routing
- ...

Key features

- Multiple interconnected views
 - list, properties, global map, local view...
- Intuitive, context-sensitive mouse-controls
- Flexible rendering style
 - SBGN support
- Semi-automated layout
 - hierarchical \Rightarrow local layout strategies

Demo



- Open model
- Zoom in, out
- Manual placement
- Browse elements
- Local views
- Cloning, branching

Work in progress...

- Support annotations (cf. biomodels.net)
- Importing/exporting rendering and layout
 - SBML rendering extension?
 - SBML layout extension supported in latest version
 - Alternative layout format: qualitative approach?
 - compact and flexible (vector graphics or CSS analogy)
 - potentially semantic driven
- Link to other tools (simulator, text mining, ...)

Concerning SBGN (1/2)

- Diagram: state transition (not sure about ER)
- S/E nodes
 - source/sink OK
 - unspecified entities only (need annotations)
 - tags? not too practical \Rightarrow “cloning glyph” instead
- Transition nodes
 - transition VS assoc/dissoc \Leftrightarrow graph topology?
 - inputs/outputs: not “centralized” at the moment

Concerning SBGN (2/2)

- Container nodes
 - Compartments: layout questions
 - nested? how do we know?
 - placing a transition node between two compartments?
 - Complex, modules: not supported at the moment
- Connecting arcs
 - consumption and production OK
 - modulation OK, but catalysis? How do we know?