

Arcadia

A visualisation tool for metabolic pathways

<http://personalpages.manchester.ac.uk/staff/Alice.Villeger/arcadia.html>

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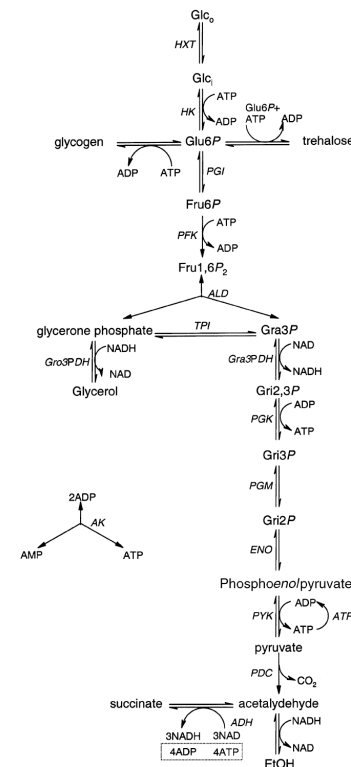
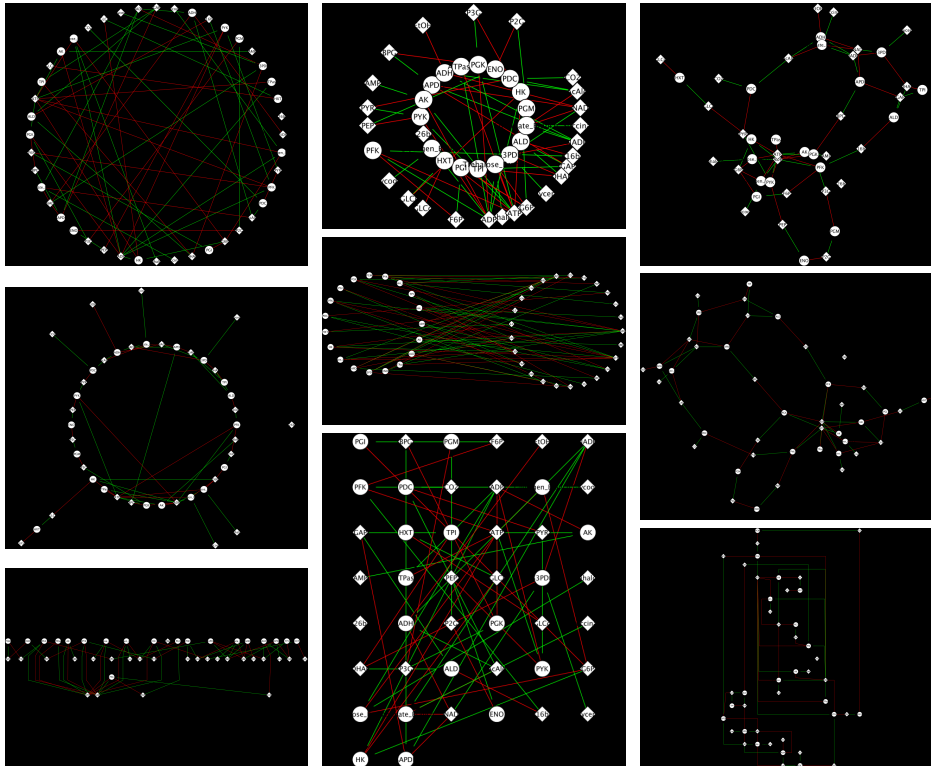
Visualising metabolic pathways

- **Network visualisation tools**
 - ✓ Allow to interactively explore **biological pathways**
 - ✓ Help **making sense** of complex systems, through:
 - **rendering** => differentiates individual **properties**
 - **layout** => emphasizes large-scale **interactions**
- **Problem: layout of metabolic pathways**
 - x **Generic** graph-drawing algorithms are inadequate
 - x Require time-consuming **manual adjustments**

Automatic VS traditional layouts

Cytoscape 2.6.0

Hand-drawn*



Layouts obtained with methods mainly designed for **protein interactions** or **signaling networks** differ significantly from the conventional representation of **metabolic pathways**

[*] Pritchard et al. 2002. "Schemes of flux control in a model of *Saccharomyces cerevisiae* glycolysis." *European Journal of Biochemistry* 269: 3894–3904.

Arcadia: a light-weight viewer

- **Viewer \neq Editor** (e.g. CellDesigner or E.P.E.)
 - **Simpler interface** with an emphasis on **navigation** between **multiple views** (= different perspectives)
- **Light-weight? => focus on interoperability**
 - Supports existing or emerging **standards** (**SBML**, SBGN)
 - **Flexible** software architecture (Model/View/Controller)
 - **Cross-platform, open-source** implementation (C++)
 - Powered by standard libraries (**LibSBML**, GraphViz, Qt, etc.)

GUI: interconnected views

The screenshot shows a software interface for a yeast glycolysis model. The window title is "[NoName] : Yeast_glycolysis_model_of_Pritchard_and_Kell". The interface is divided into three main sections:

- List View:** A table on the left showing a list of species and their neighbors. The species "ADP" is highlighted in green.
- Graphic View:** A central diagram showing a network of metabolites (F26bP, F6P, F16bP, AMP, P3C, ADP) connected by red and blue arrows. A blue box highlights this view with a list of features.
- Property View:** A bottom panel showing the properties of the selected species "ADP", including its initial amount (1.28199).

Graphic View

- ✓ zoom, scroll, drag & drop
- ✓ multiple views of a model
- x SBGN-ish style **!!**
- ✓ semi-automated layout

List View

- ✓ browse/sort/select species/reaction
- ✓ launch commands on selection

Property View

- ✓ current selection (read only)

Type	Label	Neighbours
Species	Trehalose	01
	Glycerol	01
	CO2	01
	PYR	02
	P2G	02
	NADH	04
	NAD	04
	DHAP	03
	AMP	02
	F6P	02
	G6P	04
	GLCi	02
	GLCo	01
	ATP	08
	ADP	08
	F16bP	02
	F26bP	01
	GAP	03

Species ADP
Initial Amount: 1.28199

Dynamic semi-automated layout

- **Simple controls**

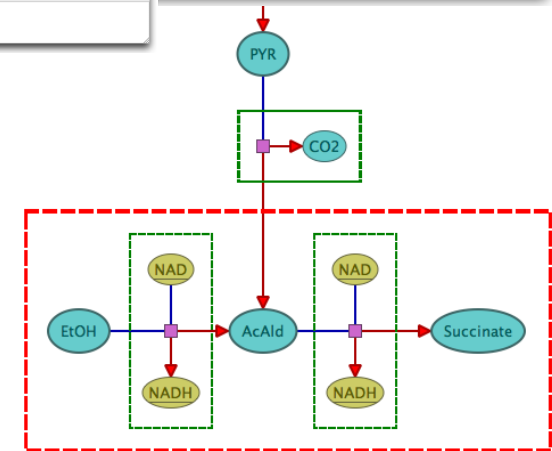
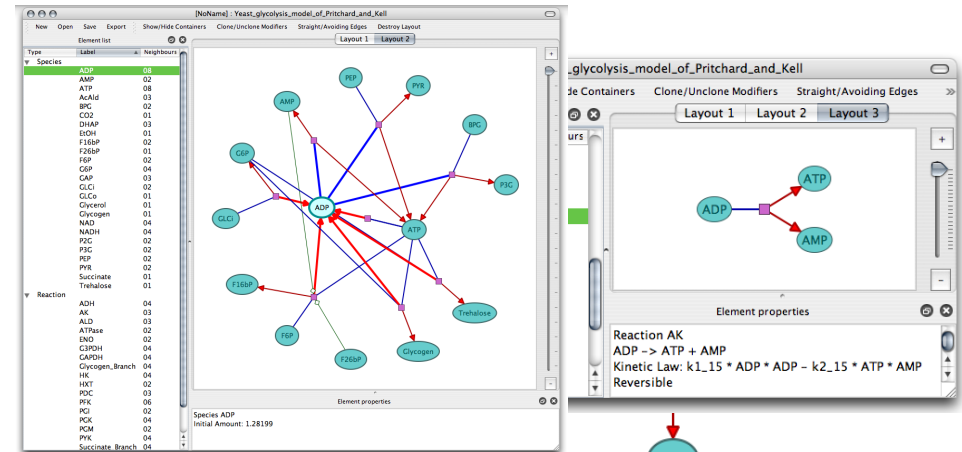
- R-click: navigate **neighbourhood** views
- 2-click: layout control

- **update** layout
- **clone** species
- **branch** reaction

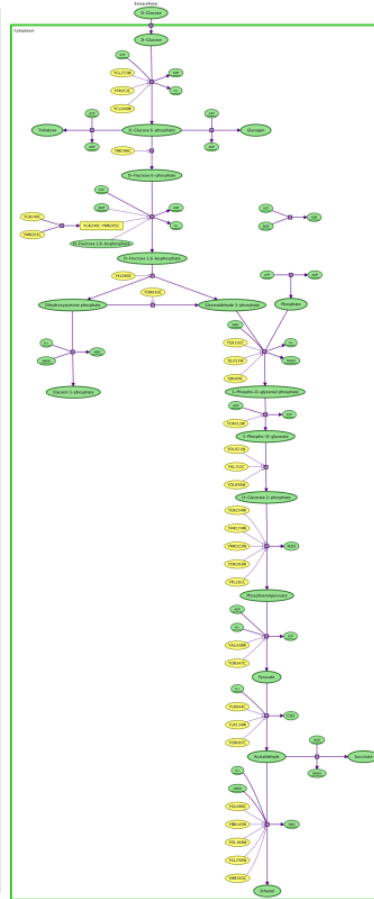
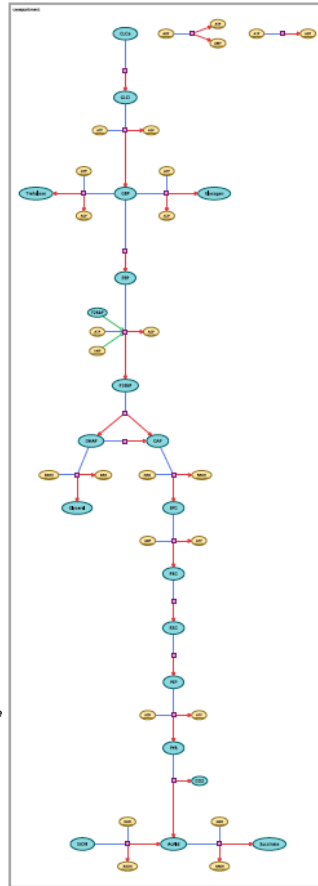
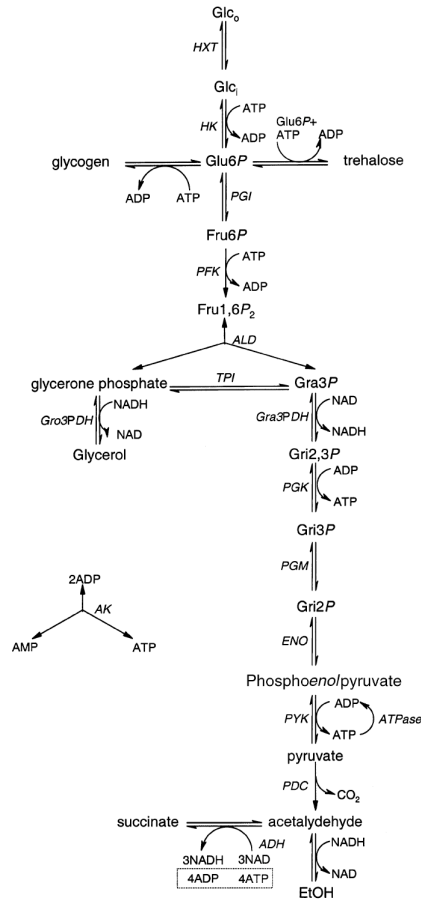
Local layout strategies

- **Menu: advanced functionalities**

→ clone all **modifiers**, merge similar reactions, ...



Layout: first results



- ✓ **prototype** tested on 10~20 models* (max. ~500 nodes)
- ✓ **semi-automated** layout similar to **hand-drawn** glycolysis diagram
- x ***work in progress*** tackling **genome-scale** models

Work in progress...

- **Graphic view**

- Full **SBGN support** (in/out reaction edges)
- expand/collapse **groups**
- advanced **navigation**

- **Other views**

- List view: **search filters**
- Property view: **edit** (and export) **annotations**

Hierarchical & progressive approach for **genome-scale** models

First release in Autumn 2008?

Data import/export

- Support of **SBML** up to L2V3

- In: **SBO** terms (\Rightarrow SBGN, property view)
 - In: **MIRIAM** annotations (\Rightarrow property view)
 - In/out: **Layout** extension ***To do*** **rendering** extension
 - In/out: proprietary annotations for dynamic layout
- } *To do* Out?

- Other formats

- Out: graphviz **graph** (dot)
- Out: **images** (bitmap and vector formats)

Subgraphs with a local layout strategy

Future plans

- Fully automated “semantic-driven” layout
 - meaningful patterns detected through **graph analysis**
 - **annotations**: e.g. subgraph = “isPartOf” group
- Interaction with other tools
 - **text mining** (REFINE project)
 - **simulation** results (SBRML)
 - Taverna workflows, as a **web service**
 - as a part of the **Utopia**^{*} framework
 - ... etc.?

[*] “UTOPIA: user friendly tools for operating informatics applications.”
Comparative and Functional Genomics 5: 56–60.

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