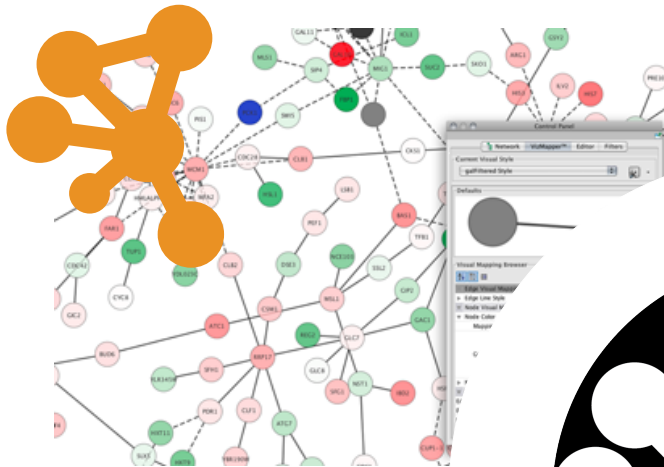


cy3sbml

Matthias König, Nicolas Rodriguez & Andreas Dräger
Charité Berlin, EMBL-EBI Hinxton, University of California, San Diego



```
<?xml version="1.0" encoding="UTF-8"?>
<model id="M1" name="M1" reversible="false">
  <listOfSpecies>
    <species id="A_out" name="A_out" boundaryCondition="true" compartment="out">
      <initialAmount value="1" unit="mole"/>
    </species>
    <species id="A_in" name="A_in" boundaryCondition="false" compartment="in">
    </species>
    <species id="B_in" name="B_in" boundaryCondition="false" compartment="in">
    </species>
    <species id="B_out" name="B_out" boundaryCondition="true" compartment="out">
    </species>
  </listOfSpecies>
  <listOfReactions>
    <reaction id="R1" name="R1" reversible="false">
      <listOfReactants>
        <speciesReference species="A_out" stoichiometry="1"/>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="A_in" stoichiometry="1"/>
      </listOfProducts>
    </reaction>
    <reaction id="R2" name="R2" reversible="false">
      <listOfReactants>
        <speciesReference species="A_in" stoichiometry="1"/>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="B_in" stoichiometry="1"/>
      </listOfProducts>
    </reaction>
  </listOfReactions>
</model>
```



cy3sbml

Problem

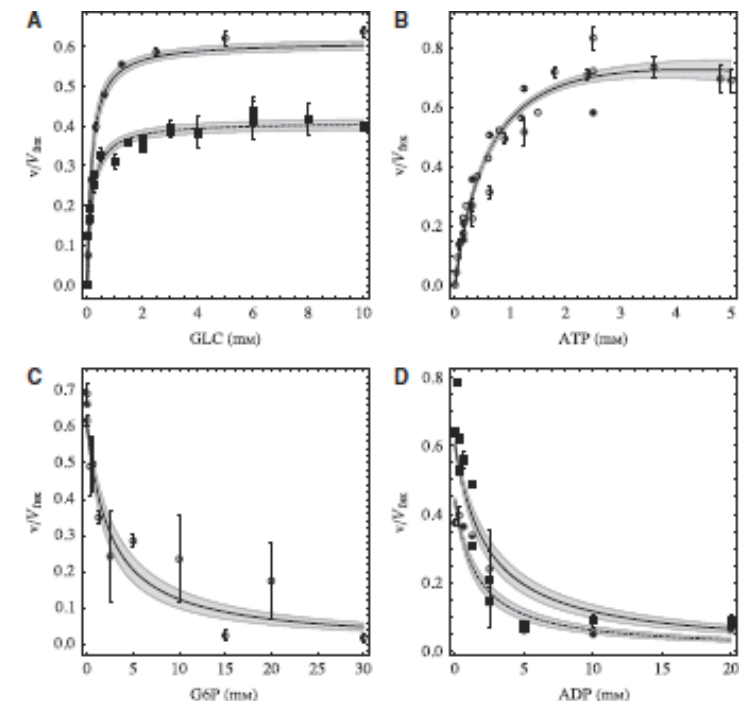
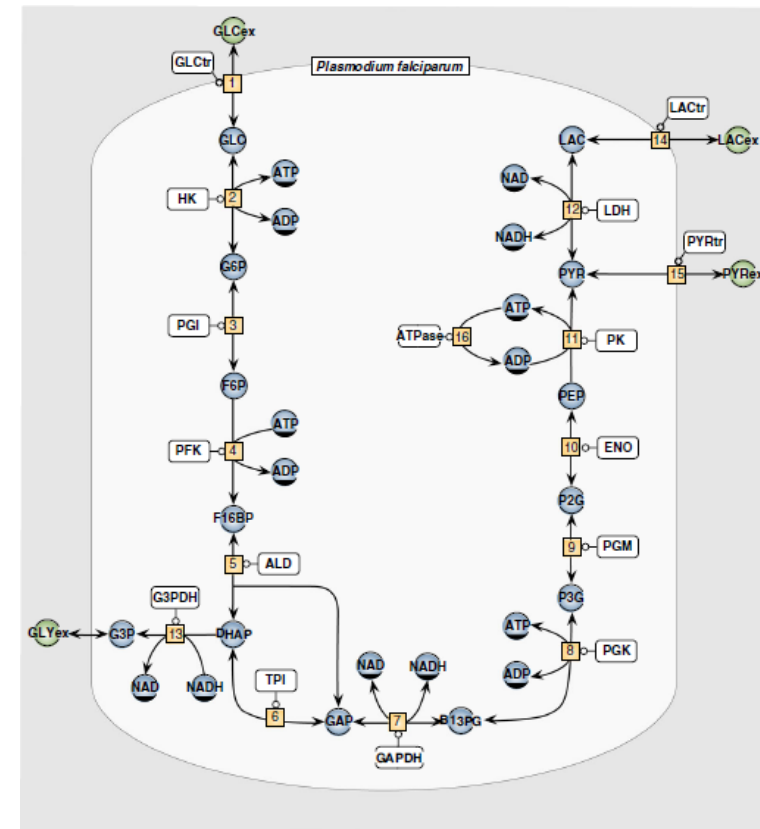
- **Current state**

- Most computational models have underlying interaction graph (metabolism, signaling, protein modification, ...)
- Multitude of modeling tools, frameworks, programming languages & workflows
- No simple visualization of models & data in the network context

- **Solution**

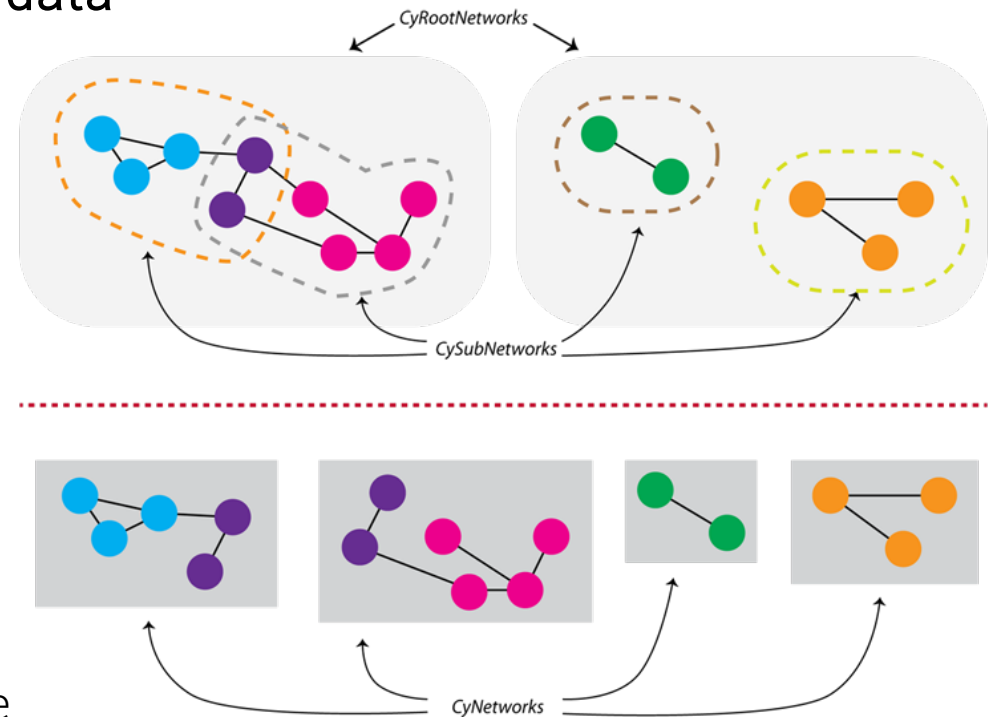
- standardized model exchange format (SBML)
- common data exchange formats (CSV, JSON)
- Easy-to-use visualization interface supporting a wide range of clients

Penkler (2015), Construction and validation of a detailed kinetic model of glycolysis in *Plasmodium falciparum*, FEBS



cy3sbml

- Cytoscape App for the **visualization of computational models & associated data in the network context**
- Porting & extending earlier work to Cytoscape 3 (König 2012, König 2010)
 - OSGI architecture (Apps & Services)
 - Hierarchical & sub-network support
 - Extended data tables
 - Node images
- Support SBML development
 - Layout, Hierarchical Models & Flux Balance
 - SBGN styles (Systems biology graphical notation)
- Small models up to genome-scale hierarchical models (~100 000 nodes)
- Support of model annotations

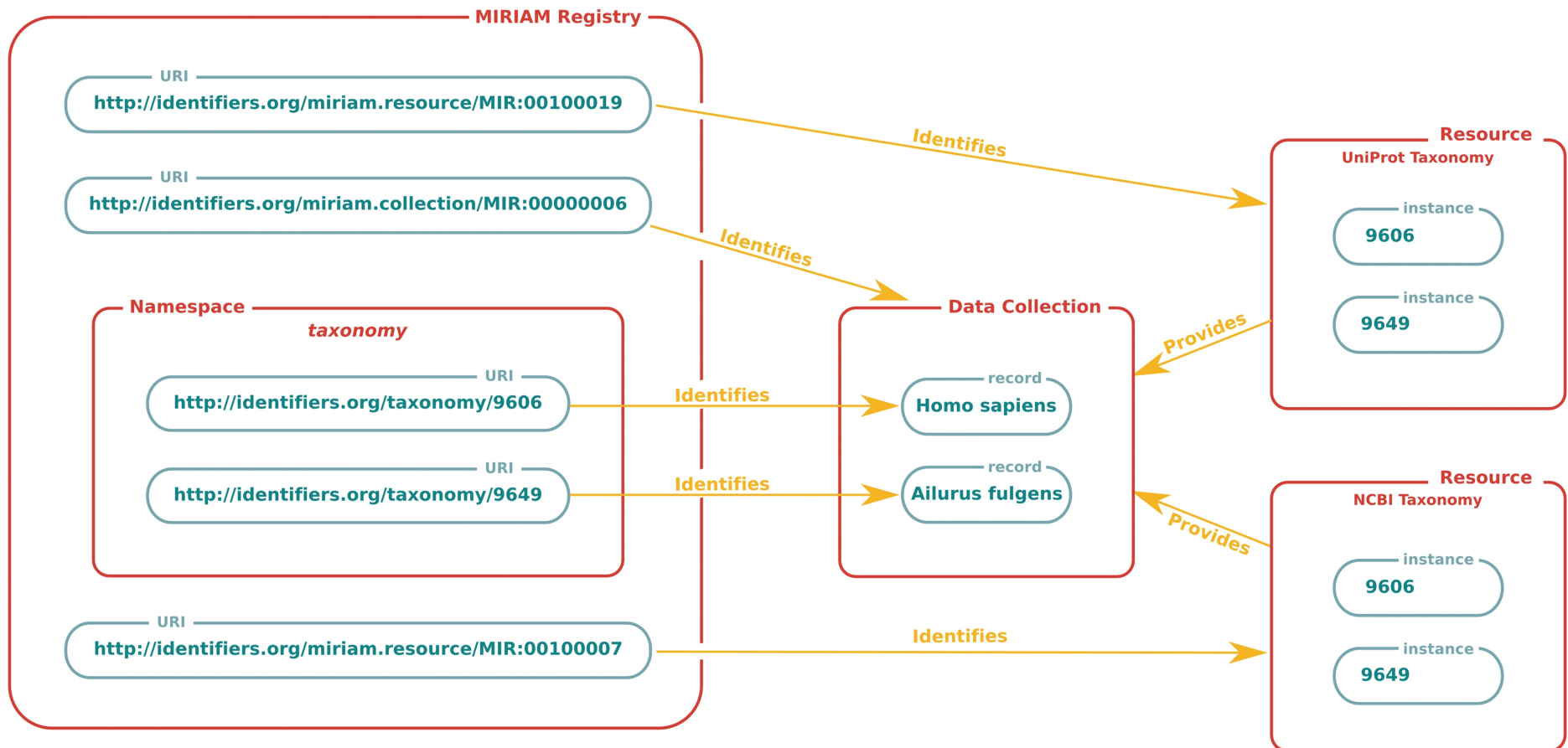


König (2012), CySBML: a Cytoscape plugin for SBML;
Bioinformatics

König (2010), FluxViz - Visualization of Flux Distributions in
Networks; Genome Informatics

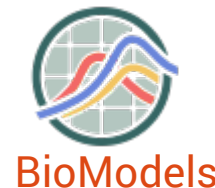
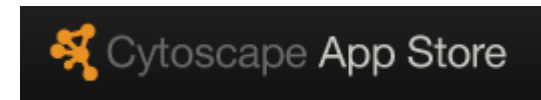
<http://chianti.ucsd.edu/cytoscape-3.2.1/API/org/cytoscape/model/package-summary.html>

RDF annotations



Integration

- Minimal requirements
 - SBML encoded model (& data with id column)
- Support wide range of clients
 - REST based API using standard exchange formats (JSON, CSV)
python, R, matlab, ...
 - Simulation libraries
 - FBA (COBRA, cobrapy)
 - Kinetic Models (RoadRunner, Copasi)
 - Gene expression networks
- Extensibility
 - cy3sbml API for additional Cytoscape Apps
- Model repositories
 - Web services & URL loading
 - BioModels
 - JWS online



Information

- **cy3sbml status**

- alpha (v0.1.3)
- first production release in 07/2015

- **Funding NRNB** (National Resource for Network Biology)

- offers the opportunity to work with open source development team on network biology related tools and resources

- **Resources**

- Open source: Code **GPLv3**, Documentation **CC BY-SA 4.0**
- Code
<https://github.com/matthiaskoenig/cy3sbml>
- Support & Forum
<https://groups.google.com/forum/#!forum/cysbml-cyfluxviz>
- Bug Tracker
<https://github.com/matthiaskoenig/cy3sbml/issues>
- Email
konigmatt@gmail.com

