# The new JWS Online simulation interface: SBGN schema generation, MIRIAM annotation and SBML model specification

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Manchester Institute for Biotechnology, University of Manchester
& JJJ group for molecular and cellular physiology
Stellenbosch University
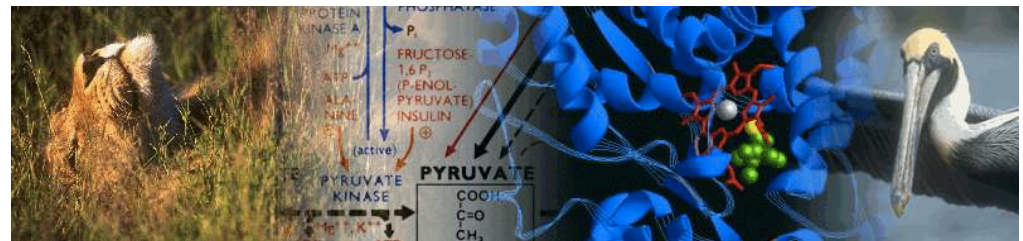
Outline

1.) What is JWS Online?

2.) JWS Online components

3.) Demonstration of new simulator

4.) Linking models and data

JWS Online

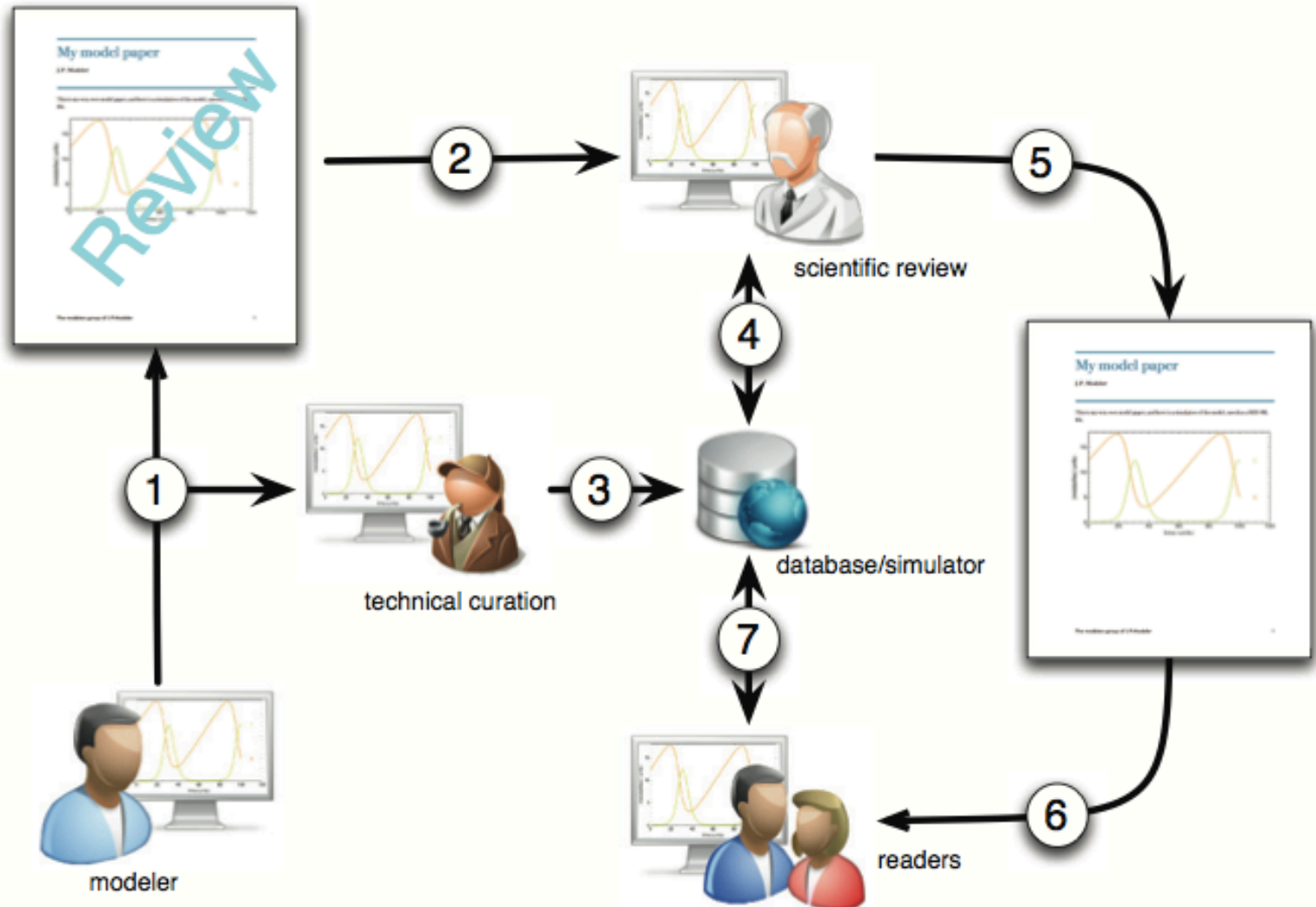- Among the first online model repositories and simulators

Repository

- Review tool for some journals
- Curated models
  - Literature
  - Direct communication
    (often as part of review process)

+ Simulable copies of BioModels

+ Private models for research groups

JWS Online
Model curation

SysMO integration

- Used by SysMO consortium
- Systems Biology of Micro-Organisms
  - Generates data for model construction
- SysMO develops a software platform:
  - **the SEEK**
    - Uses JWS Online as model simulator

the SEEK

- ## Aspects
  - ### Data capturing
    - **Bottom-up construction data**
    - **Top-down validation data**
  - ### Model simulation
  - ### Social network
- ## Goals
  - Sharing, Exchange, Reuse, Preservation of modeling research

"Find, build, describe and exchange within Systems Biology"

www.sysmo-db.org

JWS Online components

Human rea[dable]
model form[at]

Human readable model format

export

view

create edit

SBML

SBGN-ML

SBGN schema

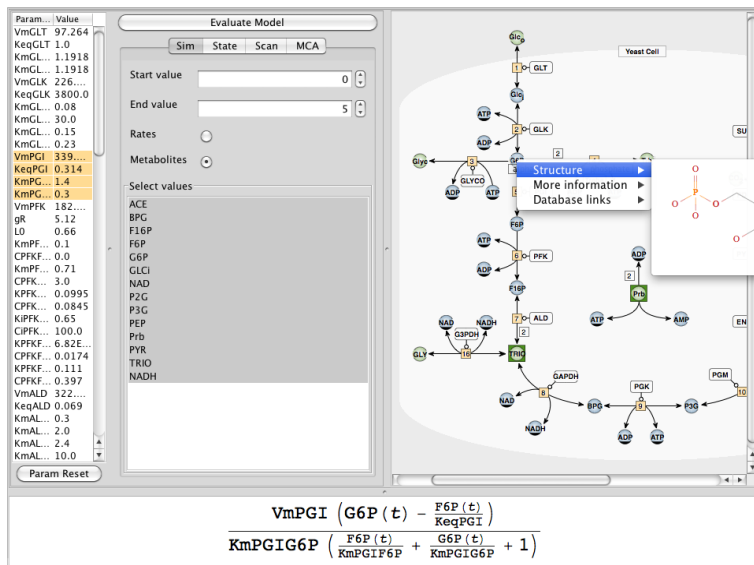**MIRIAM** annotated components

SED-ML

Stoichiometric matrices

Simulator

Web based, easy to use interface

Standard simulation functionality

Simulator upgrade

- **HTML**   **Java Applet**

  mobile friendly   security prompts

                                    loading time

- **SVG**   **GIF image**

  zoom and pan

  link to elements   link to coordinates

- **Tabbed results**   **Pop-up window**

Upload biomodel

GI

G

F

F1

NA

TR

BI

P3

P2

PI

PY

AC

NA

CPFKA

Attribution annotation ⌃

Model Name: teusink

Citation URL: http://www.bio.vu.nl,

Model URN: urn:miriam:jws:teusin

Model creators:

Given name(s): Jacky

Surname: Snoep

Email: jls@sun.ac.za

Institution: Stellenbosch Universit

Add author

Creation

Creat

Mo

Modifi

Term

webMathematica <JLink> org.sbgn.jar

```
<map>
        <glyph id="glyph9" class="macromolecule">
            <label text="vGLK"/>
            <bbox y="360.82" x="349.018" h="9.65455" w="18.0"/>
        </glyph>
        . . .
        . . .
        . . .
</map>
```

Create an error in the SBML and re-upload

```xml
<apply>
  <plus/>
  <cn type="integer"> 1 </cn>
  <apply>
    <divide/>
    <ci> F6 </ci>
    <ci> undefinedElement </ci>
  </apply>
</apply>
```

Upload altered model, OneStop outlines error
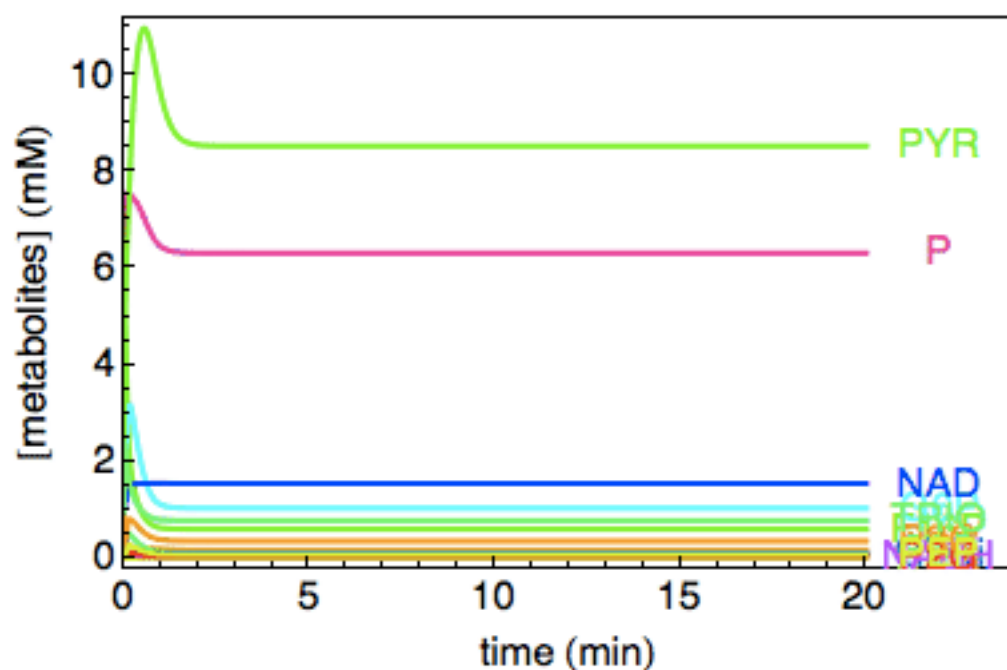
Simulation & analysis
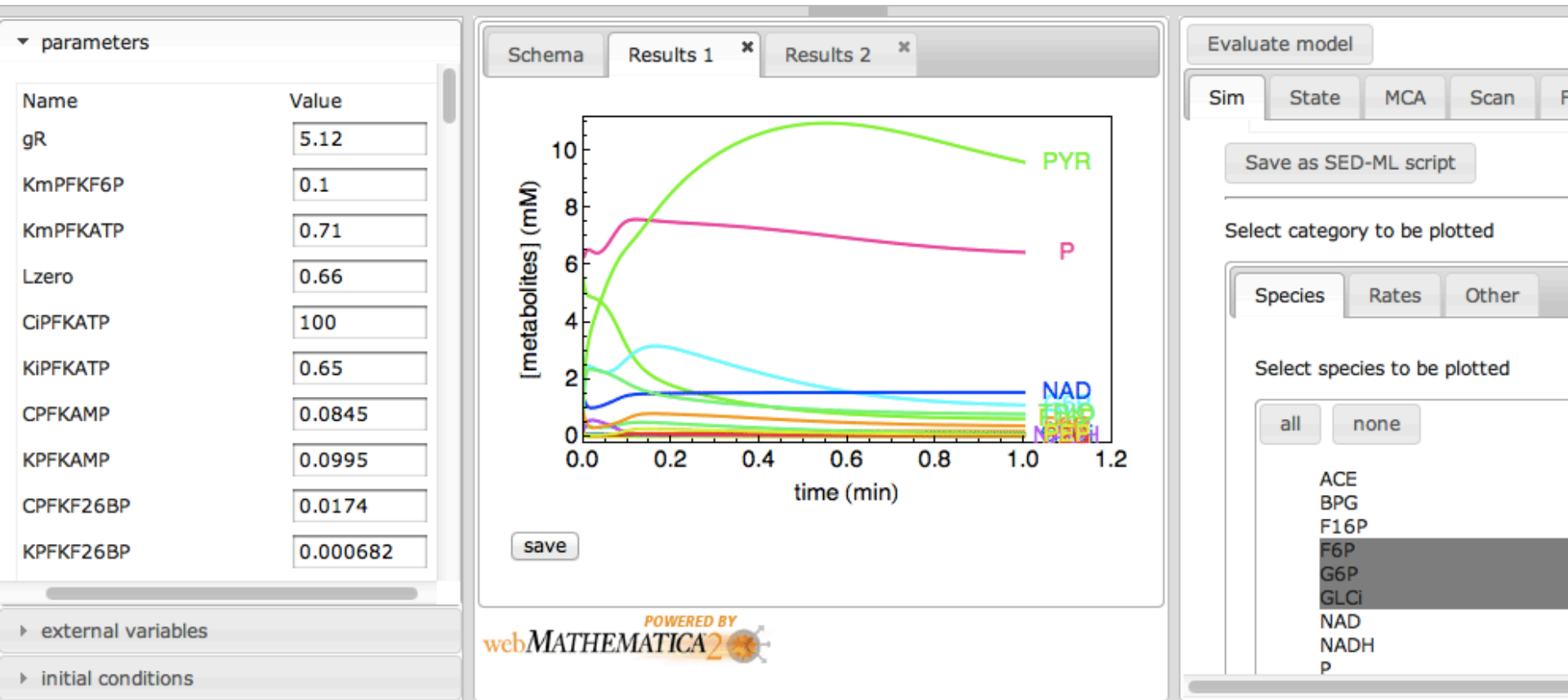
Export of SED-ML script

SED-ML simulation results:

Task: simulatebiomodel

Model: teusink

DataFuse

Goal

- Link models to
  - Construction data
  - Validation data

Find, share and exchange **Data**, **Models** and **Processes** within the SysMOOO Testing.

SysMO DB
Systems Biology of Microorganisms

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Tags [show all]

Bacillus subtilis

Biochemistry

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Computational Systems Biology

Data Management dynamics and control of biological ne...

Fermentation **Genetics**

Mathematical modelling

Matlab Microarray analysis

Microbiology

Molecular Biology ODE

parameter estimation Protein

Selected model

🚩 cronwright

🔍 View
⬇ Download

Creator: Jacky Snoep
Uploader: Jacky Snoep
Model type: Ordinary differential equations
Model format: SBML
Tags: *Not specified*

Version: 1
Associated project: SysMO-LAB
Organism: Saccharomyces cerevisiae
Environment: JWS Online

> glycerol branch

Created: 08/03/2011 @ 12:27:23 Last updated: 11/04/2011 @ 09:29:51

Selected data file

📄 Cronwright model parameter data

🌐
🔍 View
⬇ Download
🔧 Manage

Creator: Franco Du Preez
Uploader: Franco Du Preez
Tags: *Not specified*

Version: 6
Associated project: SysMO-DB

> *No description set*

Created: 29/05/2011 @ 13:28:23

Matching parameter symbols and values

ATP	F16BP	Vf1
1.39	8.01	21.0
3.56	3.96	80.0

SEEK

Find, share and exchange **Data**, **Models** and **Processes** within the SysMOOO Testing.

SysMO DB
Systems Biology of Microorganisms

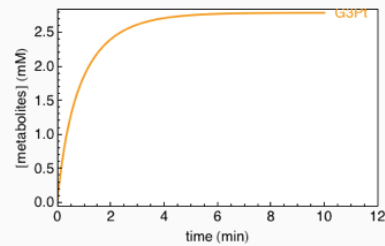| People | Projects | Institutions | Investigations | Studies | Assays | Data | Models | SOPs | Publications | Forums | Events | Help |

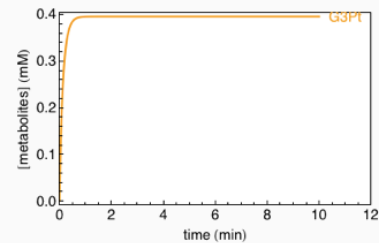[search box] All ▾ Go

simWithOrigParams

Download as CSV | View Results
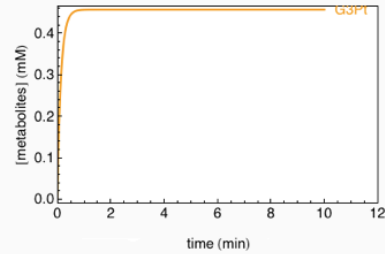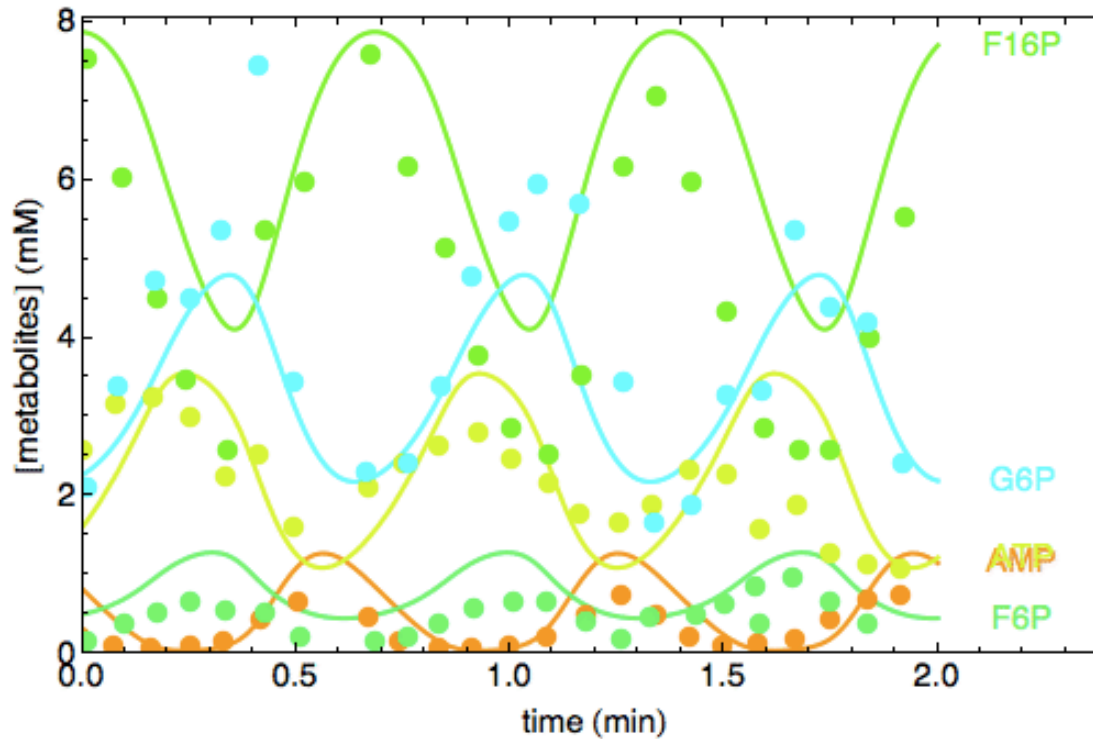

simWithExpParams1

Download as CSV | View Results

simWithExpParams2

Download as CSV | View Results

Validation data

Download the results in text or comma separated value format (e.g. for Excel import):

[Text] [CSV]

Upload data: [Choose File] no file selected   [Upload!]

Acknowledgements

- SysMO-DB team
  - Carole Goble (FBCS Manchester)
  - Stuart Owen
  - Katy Wolstencroft
  - Wolfgang Mueller (HITS)
  - Jacky Snoep (Stellenbosch)