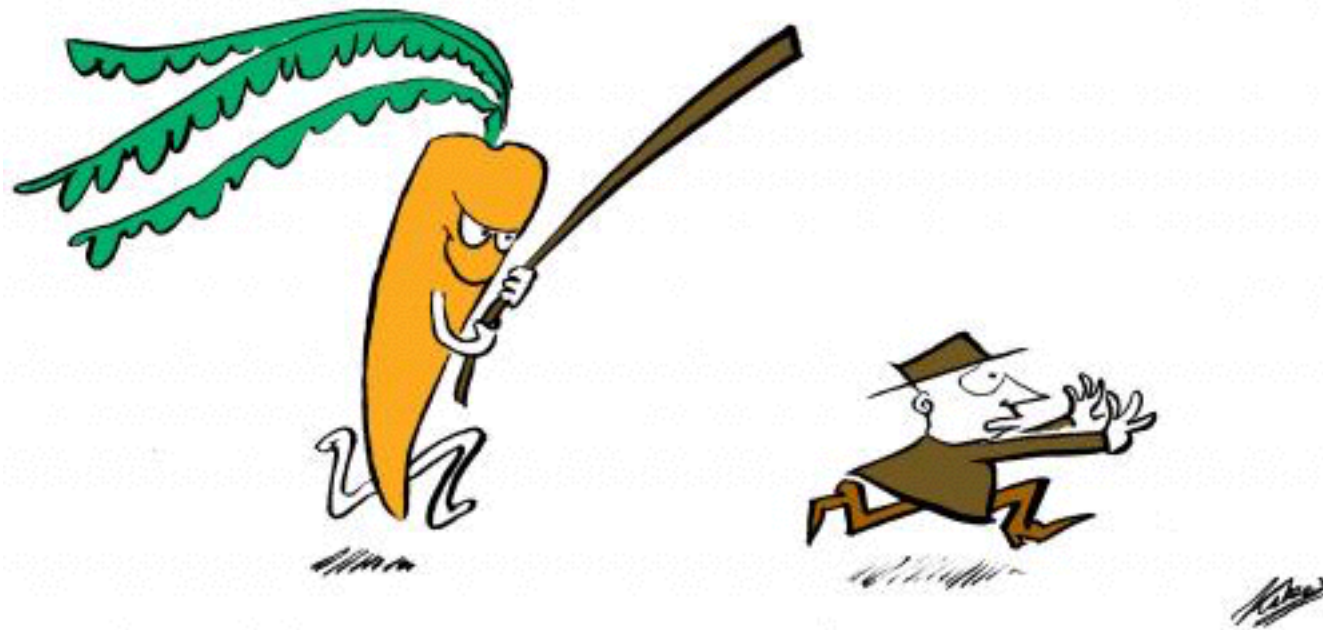


Making modelling standards more attractive to the community



J.L. Snoep, J.J. Eicher, D.D. van Niekerk, D. Waltemath,
N. Stanford, S. Owen, W. Mueller, C. Goble

Combine meeting, Salt Lake City, October 2015



Brute force



Disadvantages of stick approach to enforce standards:

- Not nice
- If scientists don't like it they will find a way around it
- Usually implemented afterwards

Make the tools so good that
sticking to standards is worth it

e.g.

If you use SBML you get good visualisation,
simulation, annotation, versioning tools.

Push to publish functionality.

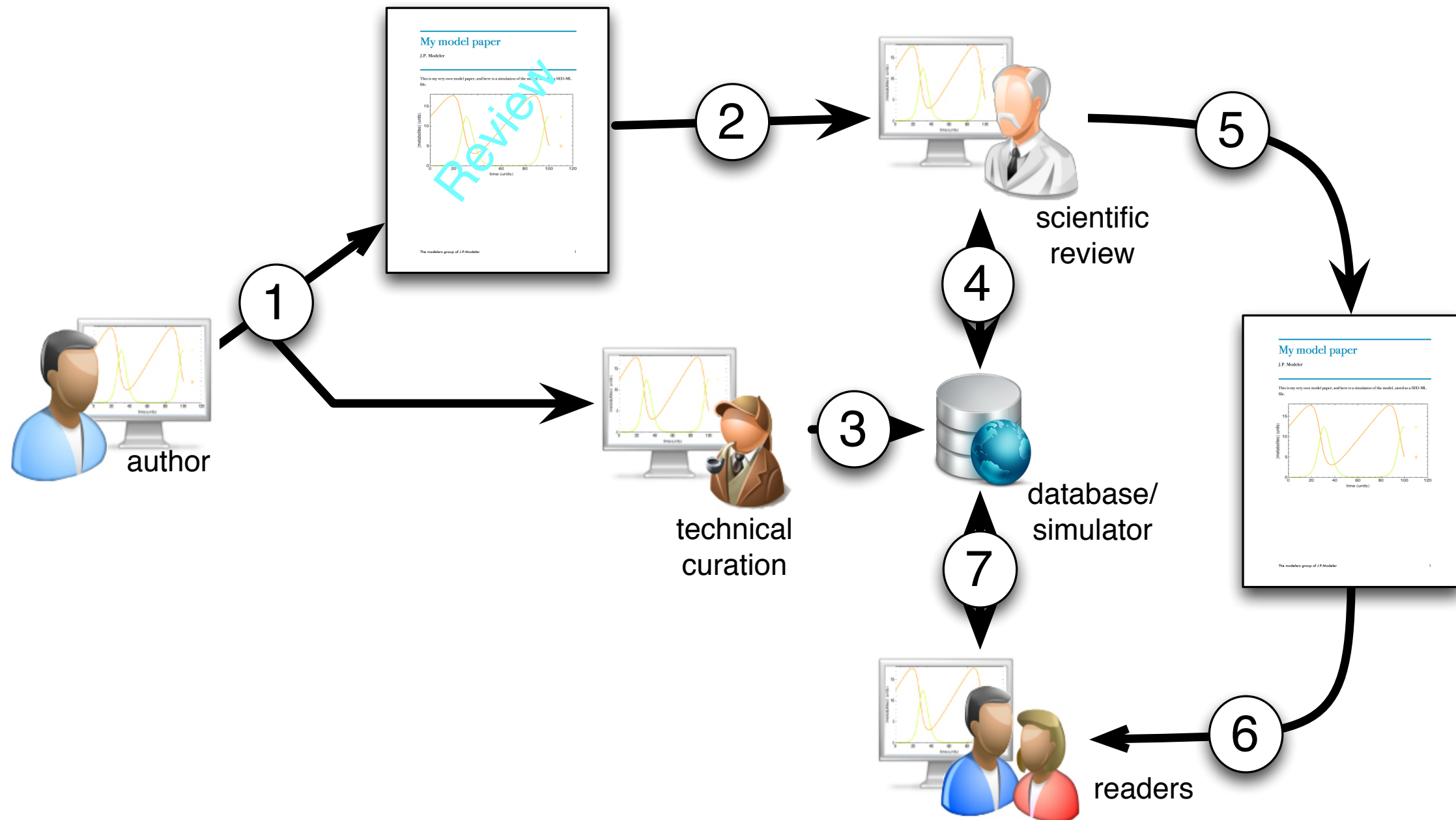
Experience with 2 types of communities

- journals, publication of mathematical models
- scientists, data and model management

What does your community want?

- scientists want to publish papers
- journals want to increase impact factor

JWS Online: link to scientific journals



FEBSJ, IET-SB, Microbiology, Metabolomics

Intermediate instability at high temperature leads to low pathway efficiency for an *in vitro* reconstituted system of gluconeogenesis in *Sulfolobus solfataricus*

Theresa Kouril¹, Dominik Esser¹, Julia Kort¹, Hans V. Westerhoff^{2,3,4}, Bettina Siebers¹ and Jacky L. Snoep^{2,3,5}

¹ Molecular Enzyme Technology and Biochemistry (MEB), Biofilm Centre, Faculty of Chemistry, University of Duisburg-Essen, Germany

² Molecular Cell Physiology, Vrije Universiteit, Amsterdam, The Netherlands

³ Manchester Centre for Integrative Systems Biology, Manchester Institute for Biotechnology, University of Manchester, UK

⁴ Synthetic Systems Biology, University of Amsterdam, Swammerdam Institute for Life Sciences, University of Amsterdam, The Netherlands

⁵ Department of Biochemistry, Stellenbosch University, Matieland, South Africa

Database

The mathematical models described here have been submitted to the JWS Online Cellular Systems Modelling Database and can be accessed at <http://jjj.mib.ac.uk/database/kouril/index.html>. The investigation and complete experimental data set is available on the SEEK at <https://seek.sysmo-db.org/investigations/51>.

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(Received 28 March 2013, revised 4 July 2013, accepted 11 July 2013)

doi:10.1111/febs.12438

phate aldolase/phosphatase, maintained a constant consumption rate of 3-phosphoglycerate and production of fructose 6-phosphate over a 1-h period. Cofactors ATP and NADPH were regenerated via pyruvate kinase and glucose dehydrogenase. A mathematical model was constructed on the basis of the kinetics of the purified enzymes and the measured half-life times of the pathway intermediates. The model quantitatively predicted the system fluxes and metabolite concentrations. Relative enzyme concentrations were chosen such that half the carbon in the system was lost due to degradation of the thermolabile intermediates dihydroxyacetone phosphate, glyceraldehyde 3-phosphate and 1,3-bisphosphoglycerate, indicating that intermediate instability at high temperature can significantly affect pathway efficiency.

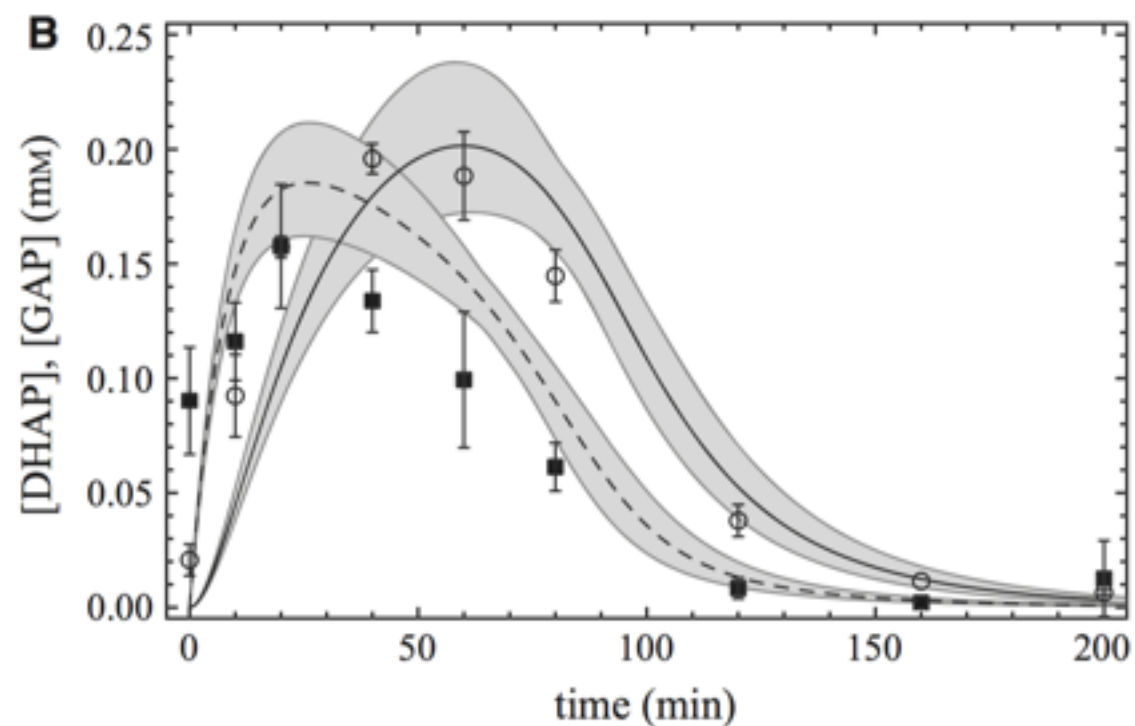
Database

The mathematical models described here have been submitted to the JWS Online Cellular Systems Modelling Database and can be accessed at <http://jjj.mib.ac.uk/database/kouril/index.html>. The investigation and complete experimental data set is available on the SEEK at <https://seek.sysmo-db.org/investigations/51>.

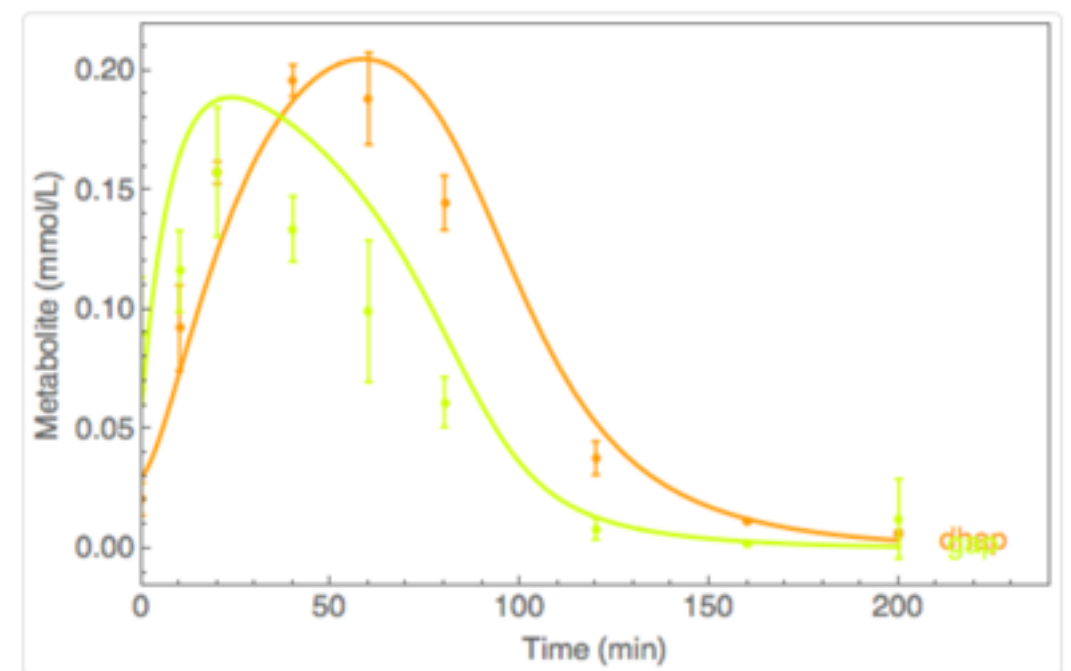
Figure in manuscript

Reproduction using SED-ML archive

Kouril et al., (2013) FEBS Journal 280: 4666–4680



[html link](#)



journal
(html)

database
(SED-ML)

simulator
(e.g. JWS)

Works for FBA models too, with a cool overlay implementation

Orth et.al., 2010 Reconstruction and Use of Microbial
Metabolic Networks. EcoSal Chapter 10.2.1

Schema

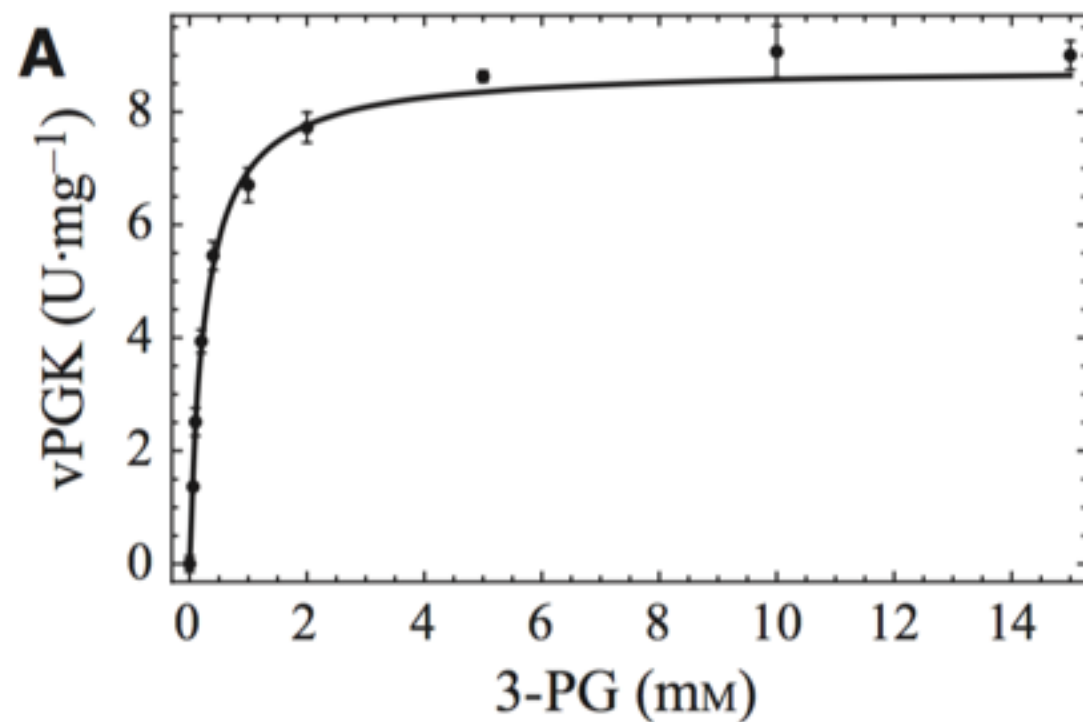
Analysis

Information



web service call

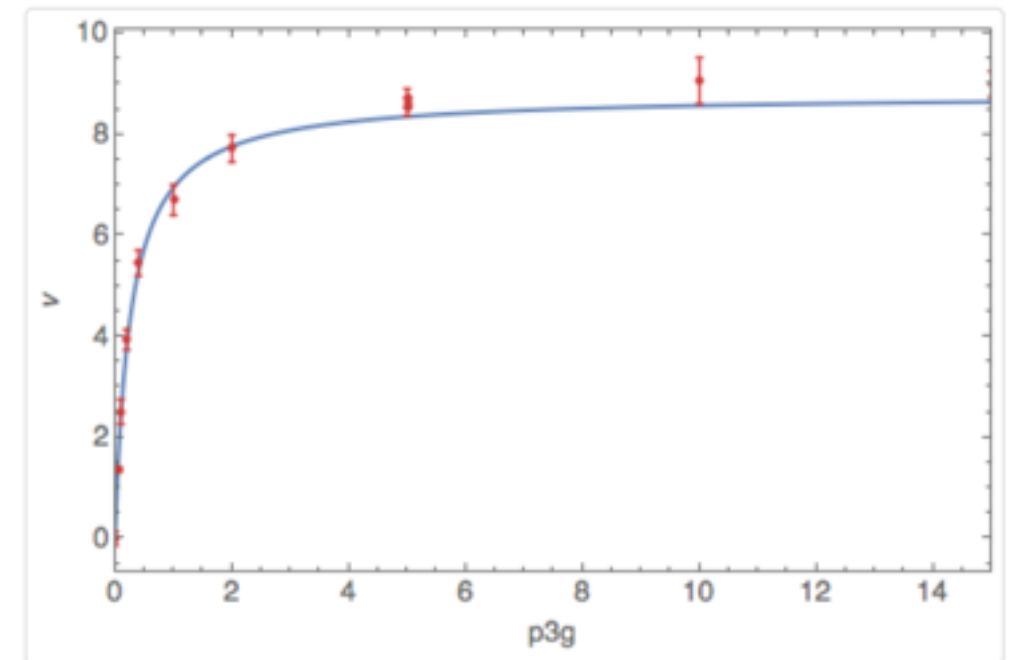
Figure in manuscript



journal
(html)

Reproduction using
web service

[html link](#)



web service

simulator
(e.g. JWS)

Data and Model Platform



SEEK: SysMO, Virtual Liver, ERASysApp, e:bio,
independent projects

<https://fairdomhub.org>

Data sharing models



Look what I've got

Data sharing models



You can have it when I am finished

Data sharing models



go for it, don't be picky

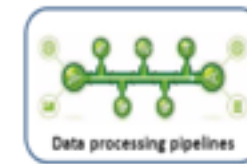
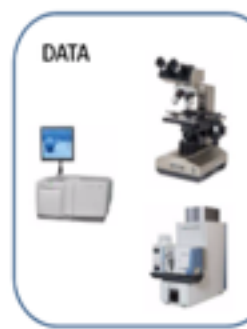
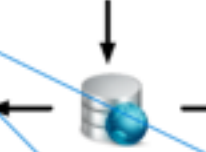
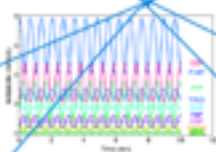
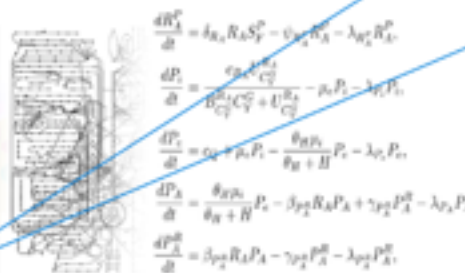
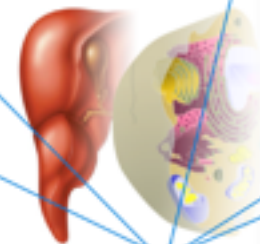
Store, index, search,
exchange, link data,
SOPs

Curate, standardise,
train assets, people

Safe repository for
assets beyond project
lifetimes

PALS knowledge
network

Publication
the wider
community



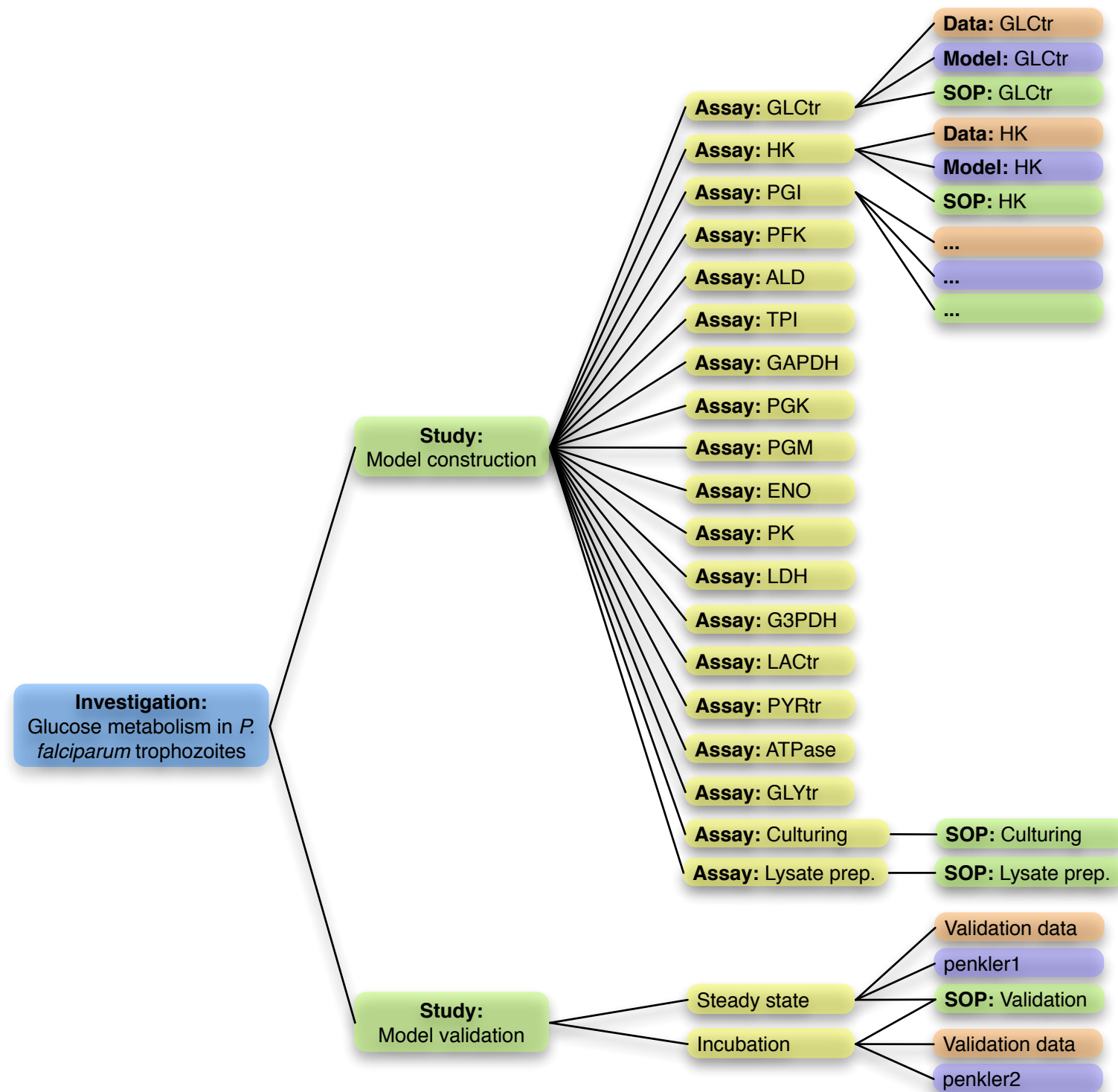
Wide adoption of
software and
methodology

Store,
index, search, exchange,
link, simulate models

Organise
investigations, studies
and assays

Sustaining curation
and support service

ISA structure in SEEK



Model file together with data reproduces the manuscript figures, parameterises the rate equations in model

Rightfield data sheets
Miriam annotated models

community interaction is crucial
if we want our tools to be used

Listen to the users, find out what they want
and make tools that address the issue

since we listen to the community

let's upload Jim's model

JWS Online
<http://jjj.bio.vu.nl>