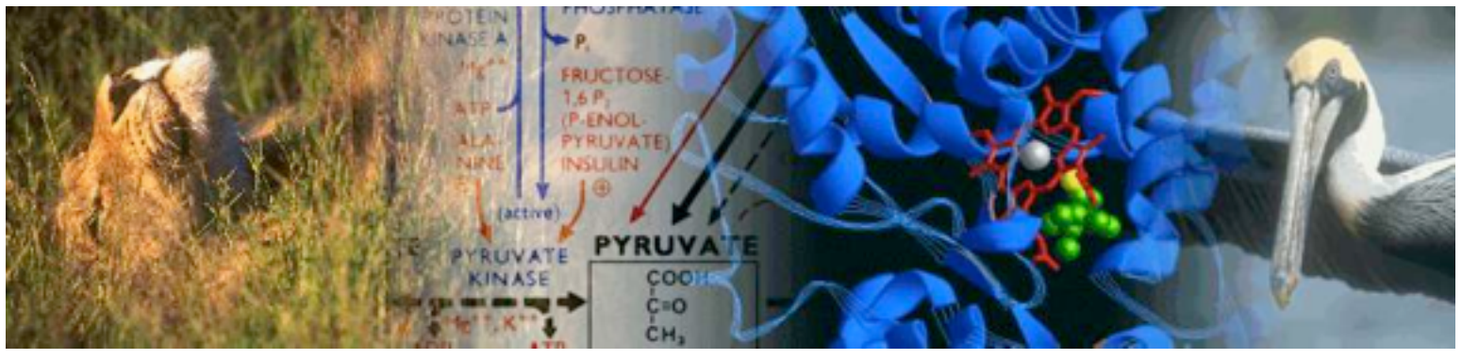


Reporting reproducible model studies; an example study using JWS Online and SEEK

Jacky L. Snoep et al.,

JWS Online team, SysMO-DB teams at Manchester and at HITS

JWS Online as a service

Review-service for scientific journals

Teaching

Collaboration with research projects

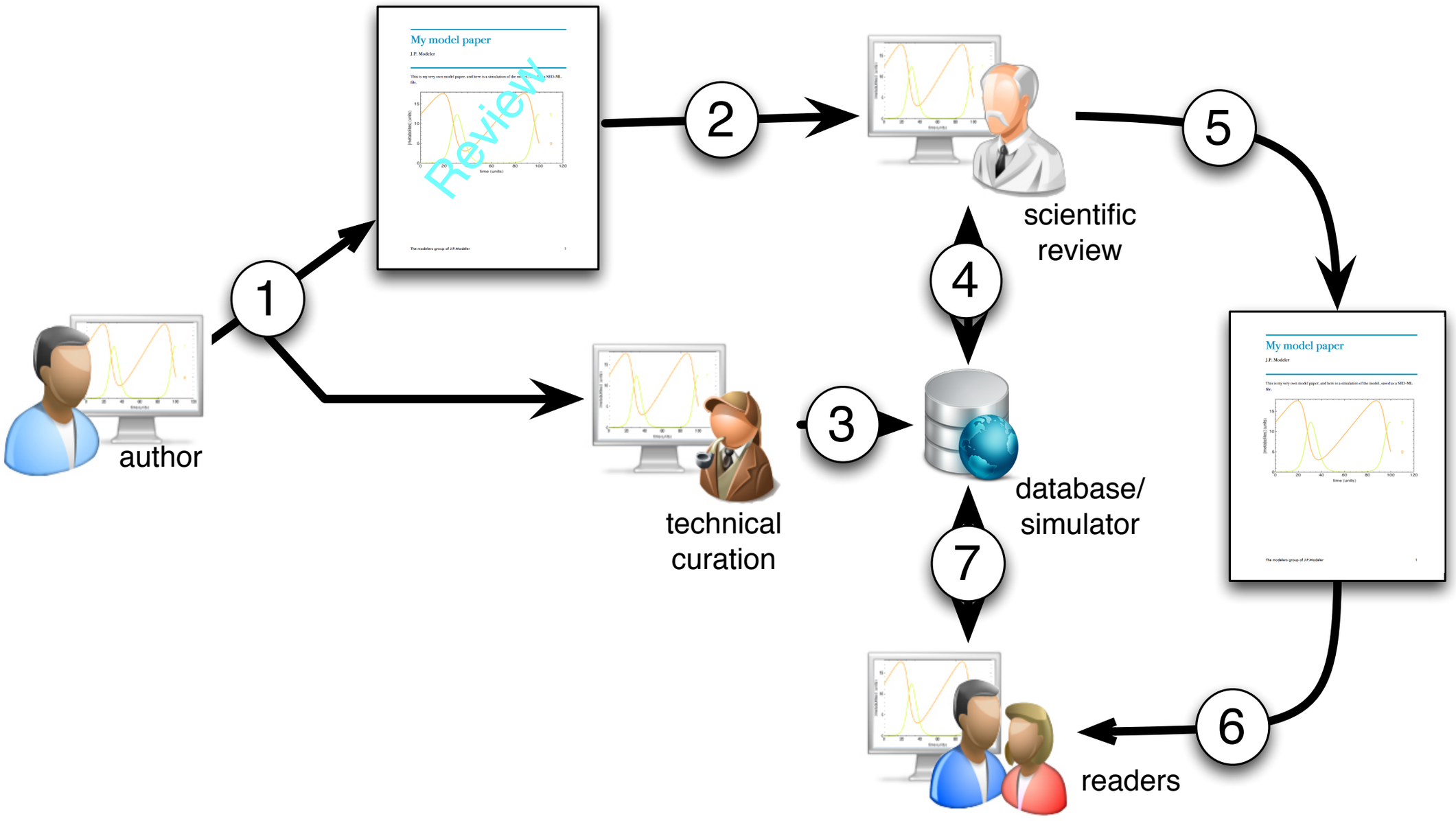
Model database
Web Simulator

Collaboration with research initiatives

Collaboration with research institutes

The Centre for Plant Integrative Biology

JWS Online: link to scientific journals



FEBSJ, IET-SB, Microbiology, Metabolomics

the FEBS Journal

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

Theresa Kouril[1], Dominik Esser[1], Julia Kort[1], Hans V. Westerhoff[2,3,4], Bettina Siebers[1] 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

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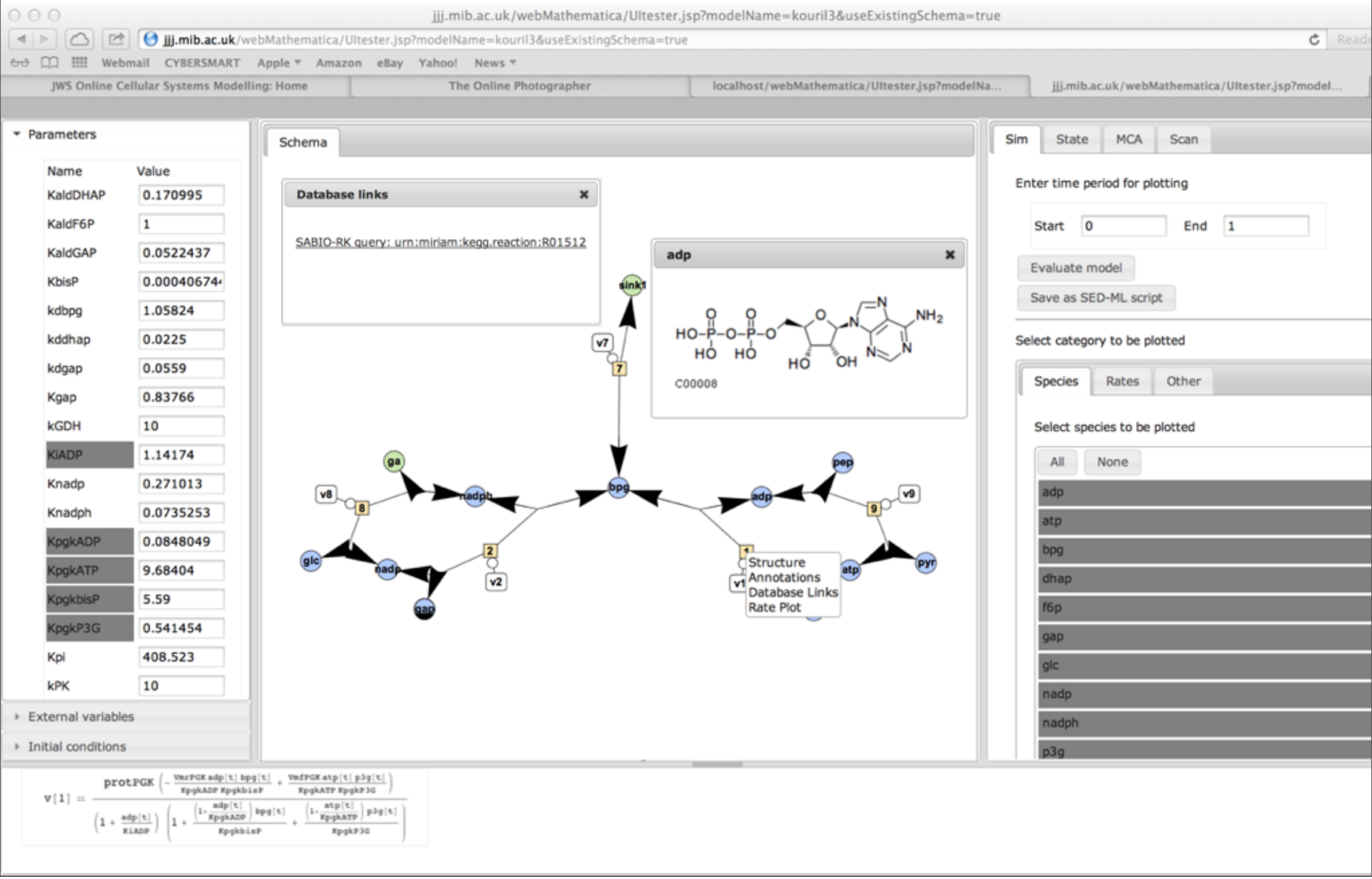
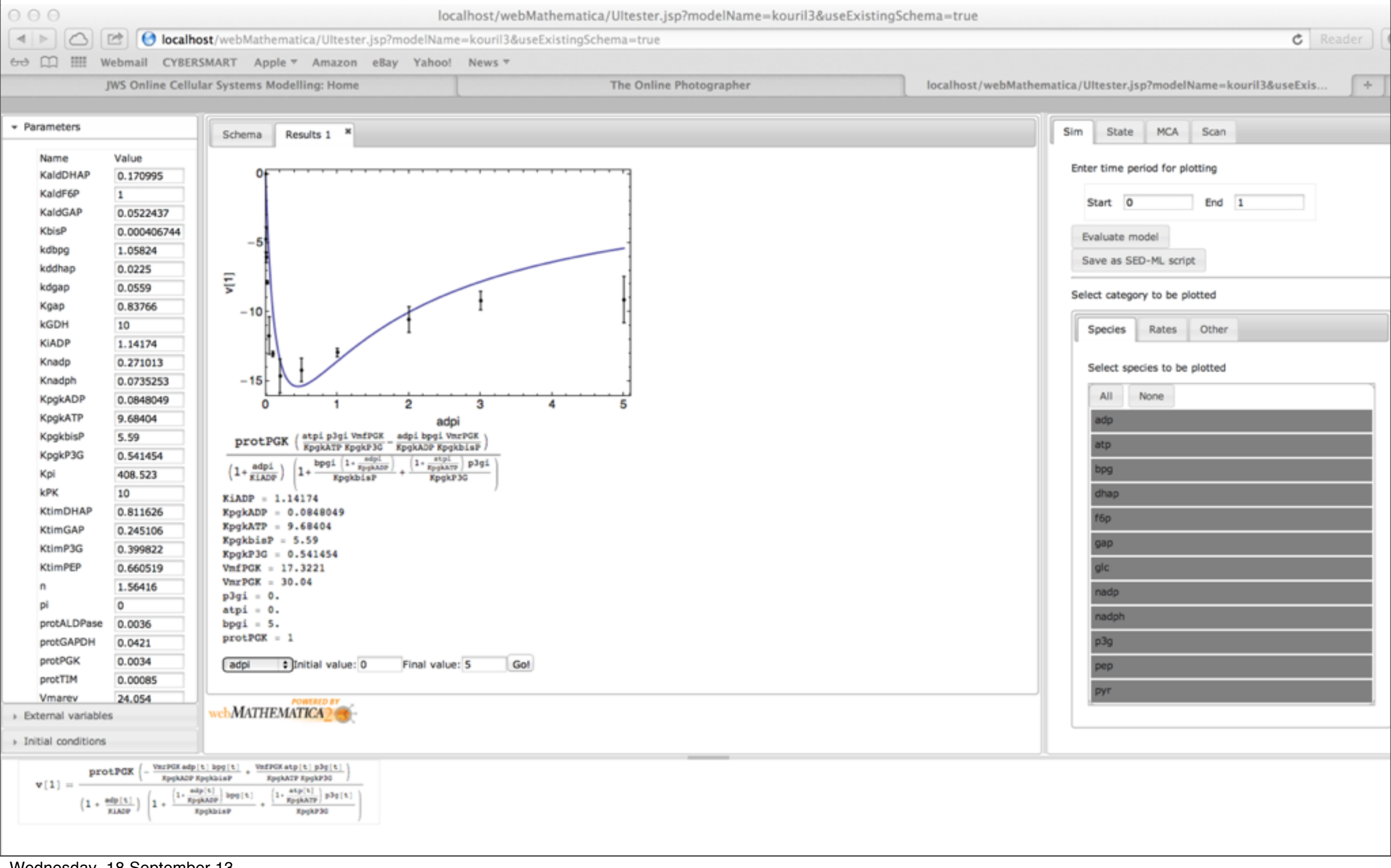
JWS Online interface



$$v[1] == \frac{\text{protPGK}\left(-\frac{\text{VmrPGK adp[t] bpg[t]}}{\text{KpgkADP KpgkbisP}} + \frac{\text{VmfPGK atp[t] p3g[t]}}{\text{KpgkATP KpgkP3G}}\right)}{\left(1 + \frac{\text{adp[t]}}{\text{KiADP}}\right)\left(1 + \frac{\left(1 + \frac{\text{adp[t]}}{\text{KpgkADP}}\right)\text{bpg[t]}}{\text{KpgkbisP}} + \frac{\left(1 + \frac{\text{atp[t]}}{\text{KpgkATP}}\right)\text{p3g[t]}}{\text{KpgkP3G}}\right)}$$

RatePLot: Isolated reaction interrogation and link to model construction data



Model simulation and link to model validation data

jjj.mib.ac.uk/webMathematica/Ultester.jsp?modelName=kouril3&useExistingSchema=true

jjj.mib.ac.uk/webMathematica/Ultester.jsp?modelName=kouril3&useExistingSchema=true

Webmail CYBERSMART Apple Amazon eBay Yahoo! News

JWS Online Cellular Systems Modelling: Home | The Online Photographer | localhost/webMathematica/Ultester.jsp?modelNa... | jjj.mib.ac.uk/webMathematica/Ultester.jsp?model...

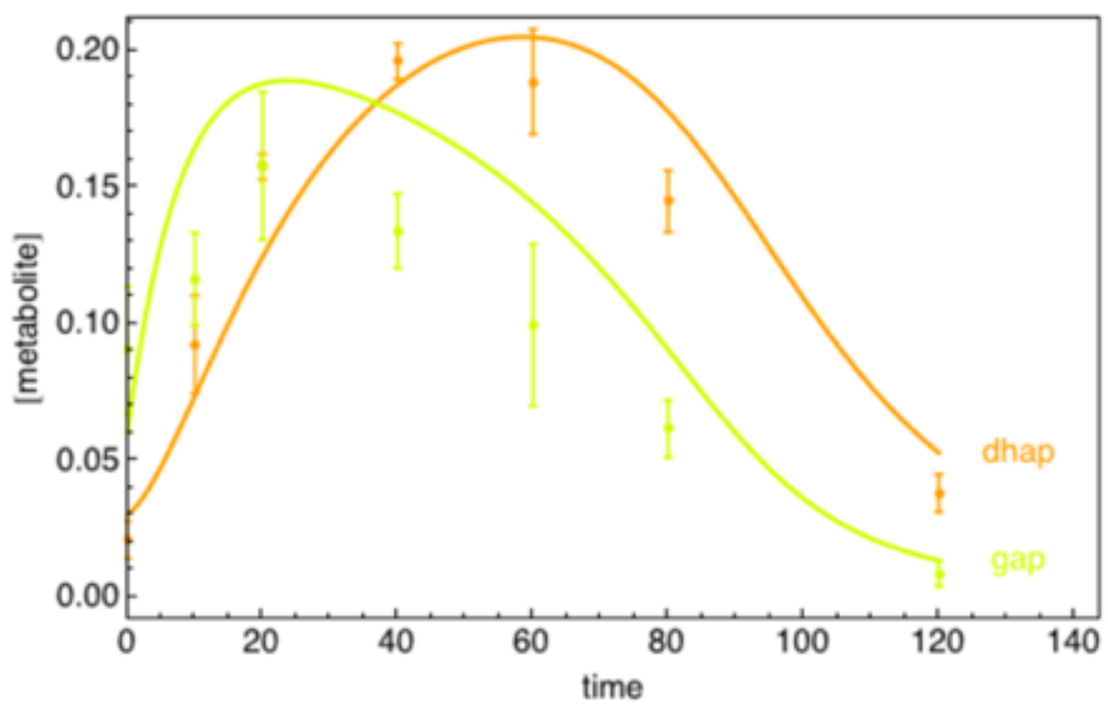
Parameters

Name	Value
KaldDHAP	0.170995
KaldF6P	1
KaldGAP	0.0522437
KbisP	0.000406744
kdbpg	1.05824
kddhap	0.0225
kdgap	0.0559
Kgap	0.83766
kGDH	10
KiADP	1.14174
Knadp	0.271013
Knadph	0.0735253
KpgkADP	0.0848049
KpgkATP	9.68404
KpgkbisP	5.59

External variables

Initial conditions

Schema | Results 2 | Results 3



Save as CSV

POWERED BY webMATHEMATICA 2

Sim | State | MCA | Scan

Enter time period for plotting

Start 0 End 120

Evaluate model

Save as SED-ML script

Select category to be plotted

Species | Rates | Other

Select species to be plotted

All | None

adp

atp

bpg

dhap

f6p

gap

$$v[1] = \frac{\text{protPGK}\left(-\frac{\text{VmrPGK adp[t] bpg[t]}}{\text{KpgkADP KpgkbisP}} + \frac{\text{VmfPGK atp[t] p3g[t]}}{\text{KpgkATP KpgkP3G}}\right)}{\left(1+\frac{\text{adp[t]}}{\text{KiADP}}\right)\left(1+\frac{\left(1+\frac{\text{adp[t]}}{\text{KpgkADP}}\right)\text{bpg[t]}}{\text{KpgkbisP}} + \frac{\left(1+\frac{\text{atp[t]}}{\text{KpgkATP}}\right)\text{p3g[t]}}{\text{KpgkP3G}}\right)}$$

SED-ML output and simulation

Schema | Results 2 | Results 3 | Results 4

SED-ML script to reproduce the simulation:

```
<?xml version="1.0" encoding="utf-8"?>
        <sedML xmlns:math="http://www.w3.org/1998/Math/MathML" xmlns="http://sec
level="1" version="1">
        <listOfSimulations>
        <uniformTimeCourse  initialTime="0.0" numberOfPoints="100" outputStartTime=
outputEndTime="120" id="utc1">
        <algorithm kisaoID="KISAO:0000365" />
        </uniformTimeCourse>
        </listOfSimulations>
        <listOfModels>
        <model id="model1" name="urn:miriam:jws:kouril3" source="urn:miriam:jws:kou
language="urn:sedml:language:sbml.level-2.version-3" >
<listofchanges><changeattribute target="KaldDHAPJWSparam" newvalue="0.170995">
</changeattribute><changeattribute target="KaldF6PJWSparam" newvalue="1">
</changeattribute><changeattribute target="KaldGAPJWSparam" newvalue="0.05224
</changeattribute><changeattribute target="KbisPJWSparam" newvalue="0.00040674
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</changeattribute><changeattribute target="kddhapJWSparam" newvalue="0.0225">
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</changeattribute><changeattribute target="kGDHJWSparam" newvalue="10"></char
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<changeattribute target="KpgkATPJWSparam" newvalue="9.68404"></changeattribut
<changeattribute target="KpgkbisPJWSparam" newvalue="5.59"></changeattribute>
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<changeattribute target="KpiJWSparam" newvalue="408.523"></changeattribute>
<changeattribute target="kPKJWSparam" newvalue="10"></changeattribute><change
target="KtimDHAPJWSparam" newvalue="0.811626"></changeattribute><changeattri
```

Sim | State | MCA | Scan

Enter time period for plotting

Start 0 End 120

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Save as SED-ML script

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Select species to be plotted

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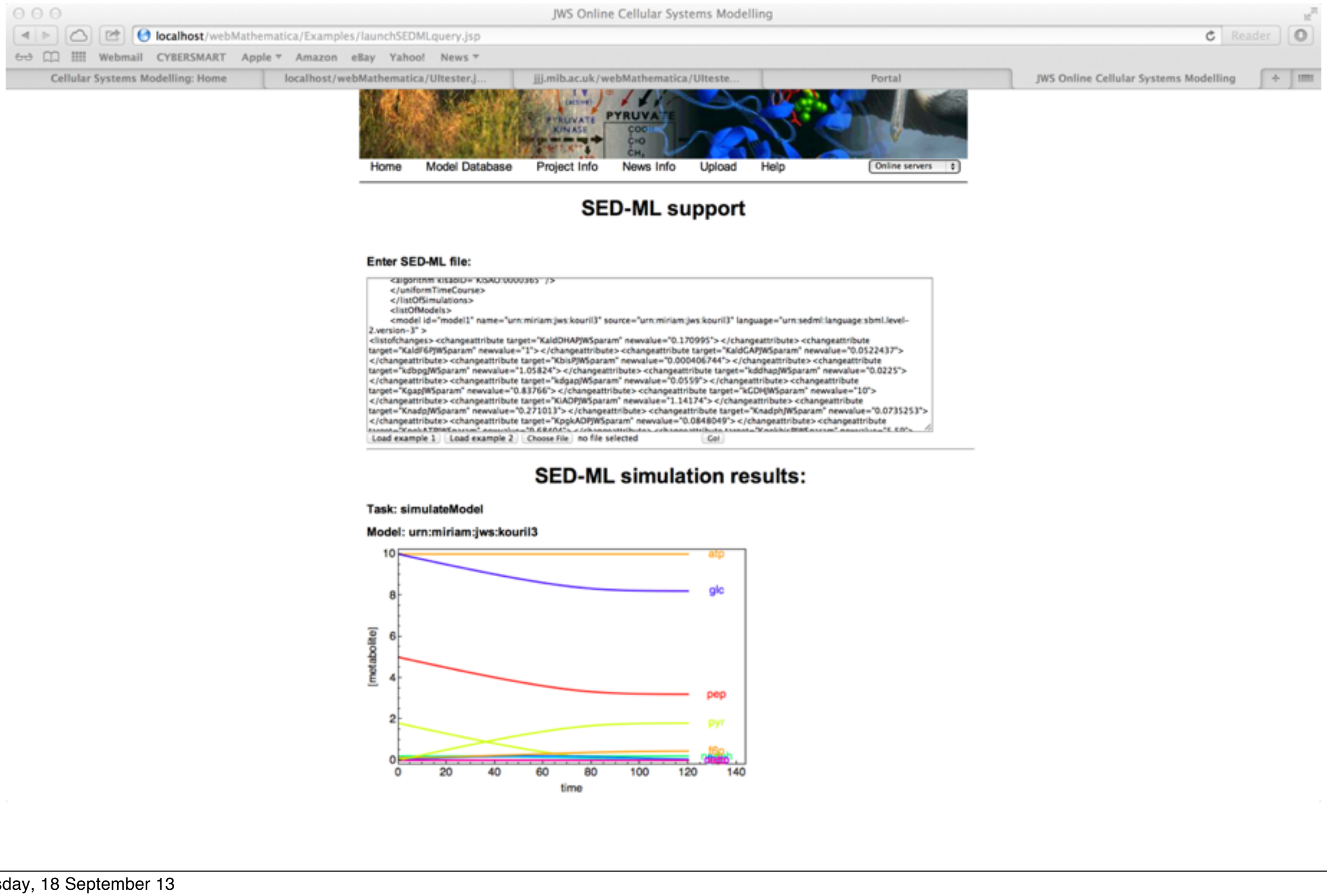
- dhap
- f6p
- gap

SED-ML output and simulation (launchSEDMLquery.jsp)



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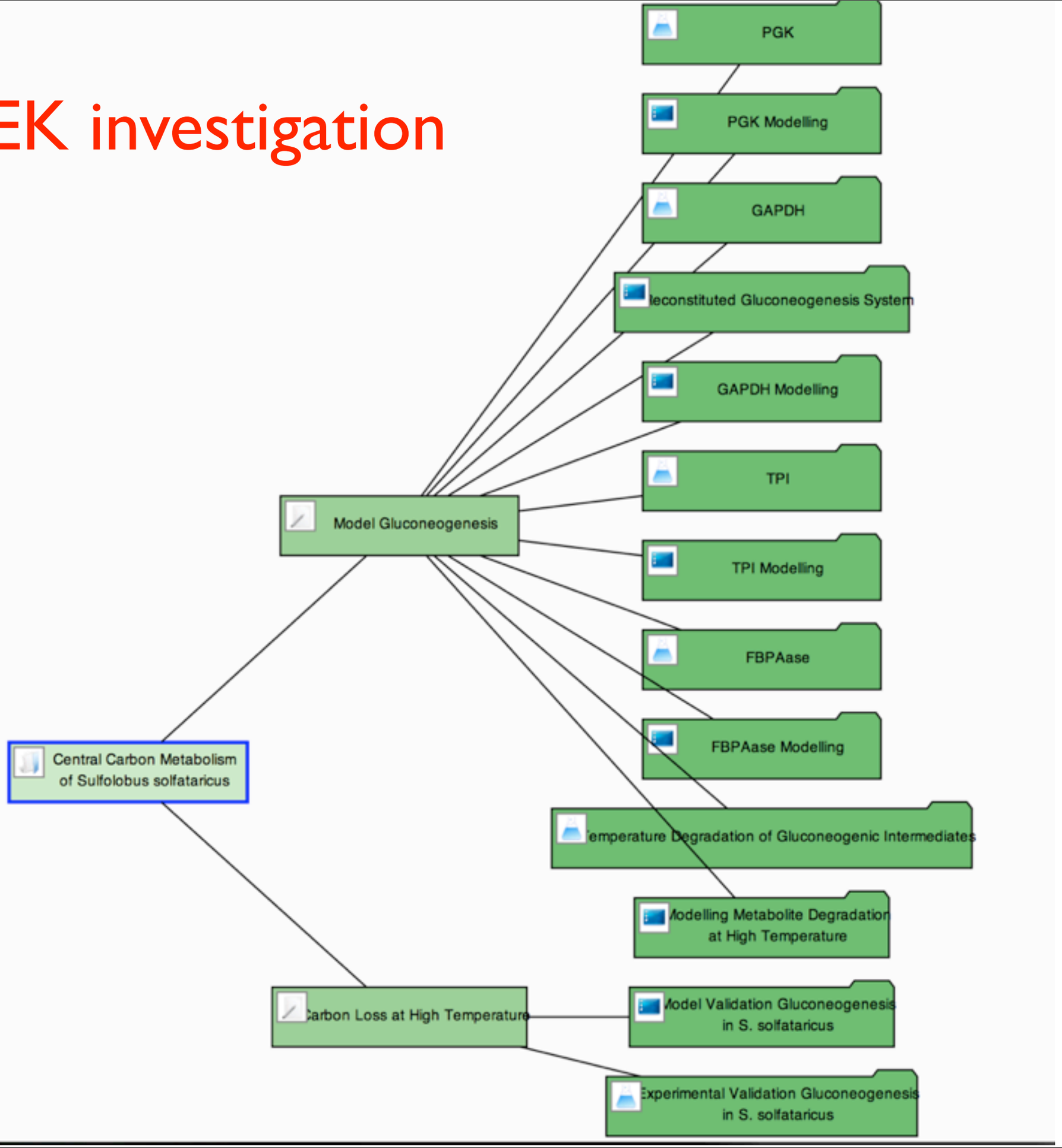
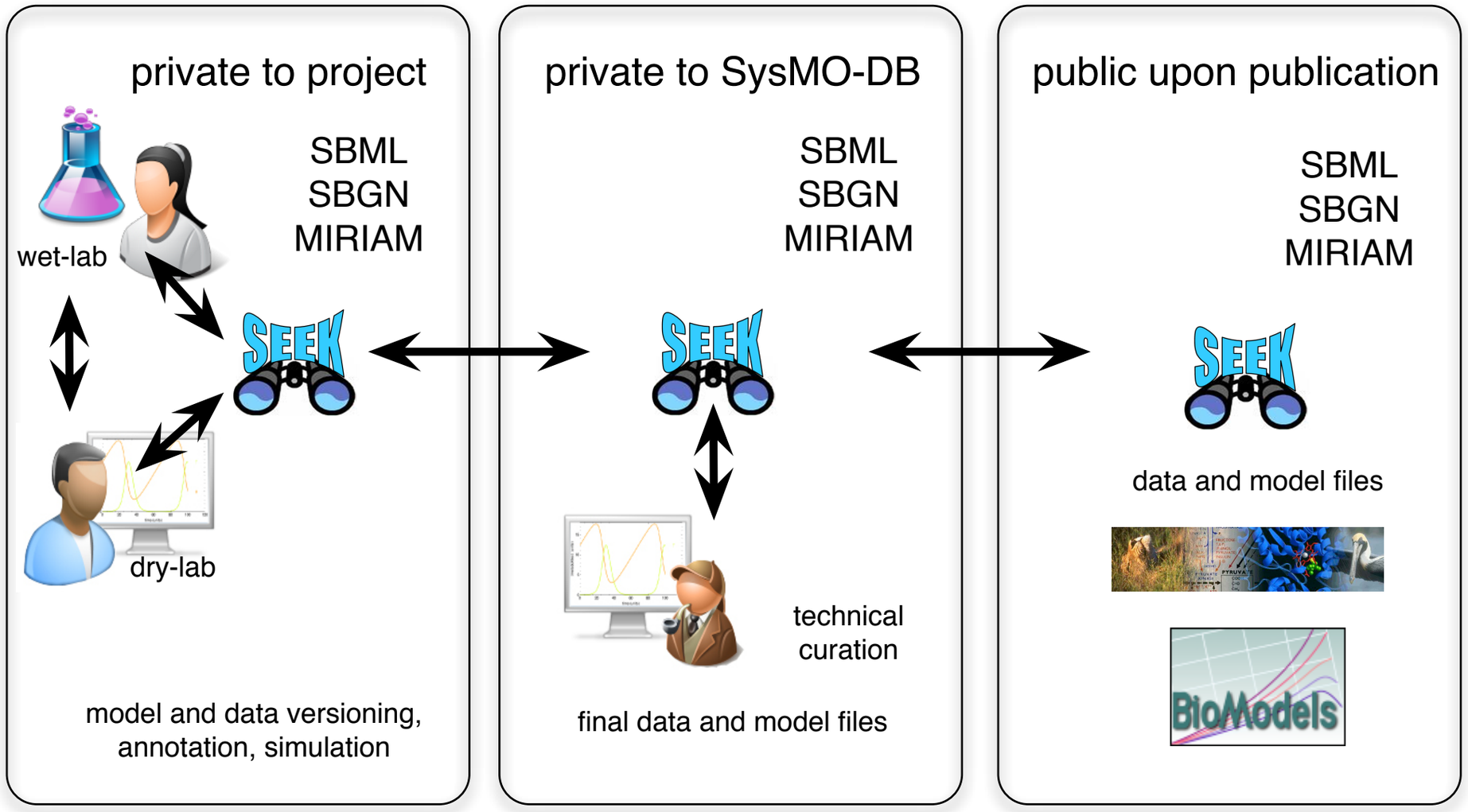
SEEK investigation



JWS Online: link to SEEK/projects



Thank you!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National Research Foundation
RISA
Research and Innovation Support and Advancement


SysMO
Systems Biology of Microorganisms


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