E-cyanobacterium.org

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Systems Biology Laboratory
Masaryk University Brno

CMSB 2016, University of Cambridge, UK

23 September 2016

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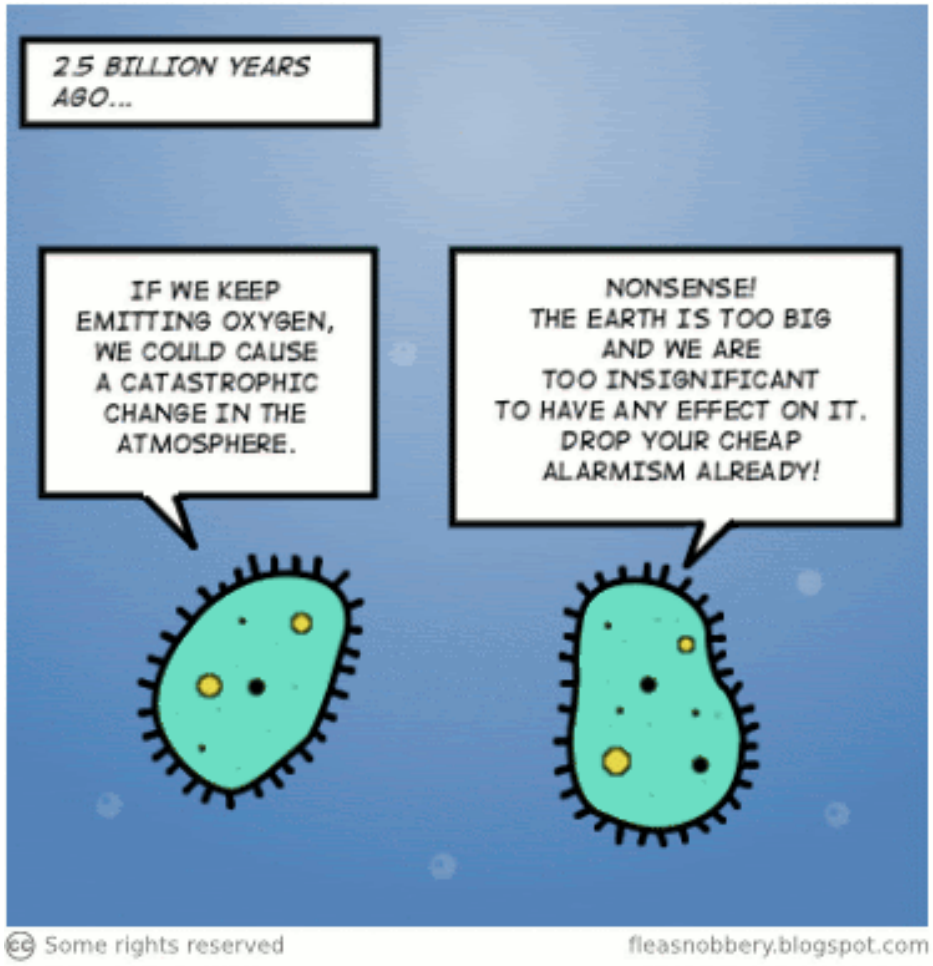

CyanoTeam, Reg. No. CZ.1.07/2.3.00/20.0256
National Infrastructure for Systems Biology, C4SYS

Background

Domain-Specific Modelling Platform

- systems biology consortium focused on a specific problem
  - cyanobacteria in various environments
- collaborative development of models
  - identify the processes at a sufficient level of abstraction
  - collect existing and create new dynamical models
  - project models onto the unified biochemical space
- supply experimental data for model validation
- generally aimed tools do not give satisfactory support (Biomodels.net, Opencell.org, JWS Online,...)

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Web-based Platform for Systems Biology of Cyanobacteria

- interactive **online platform** for cyanobacteria processes
- unified standard format (SBML) supplied with **uniform annotation** that is executable
- full understanding, re-using, and comparing of models
- storage, maintenance and presentation of experimental data
- content visualisation

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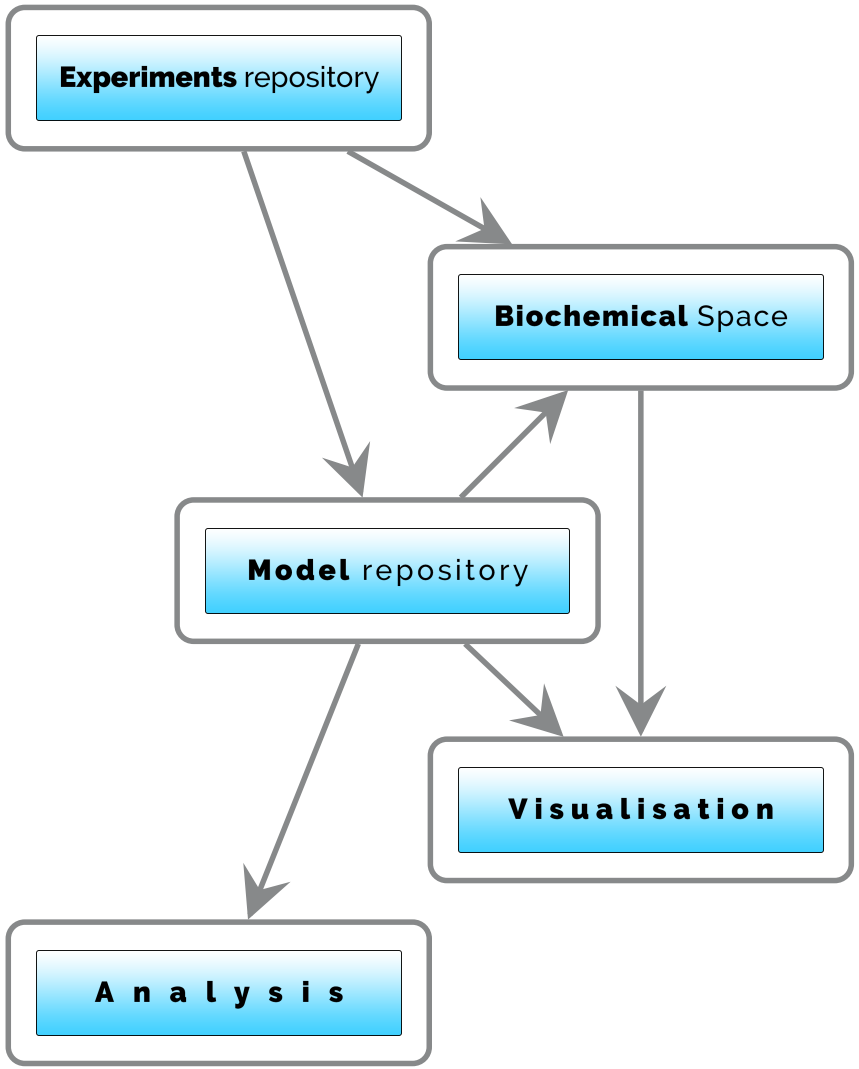
Overview

- modular design
- aim to make the integration tighter



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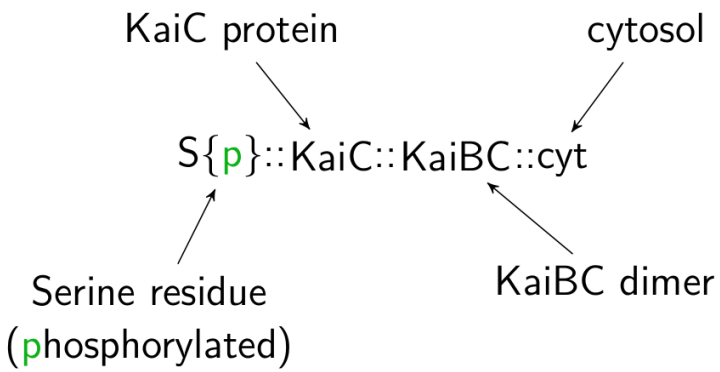
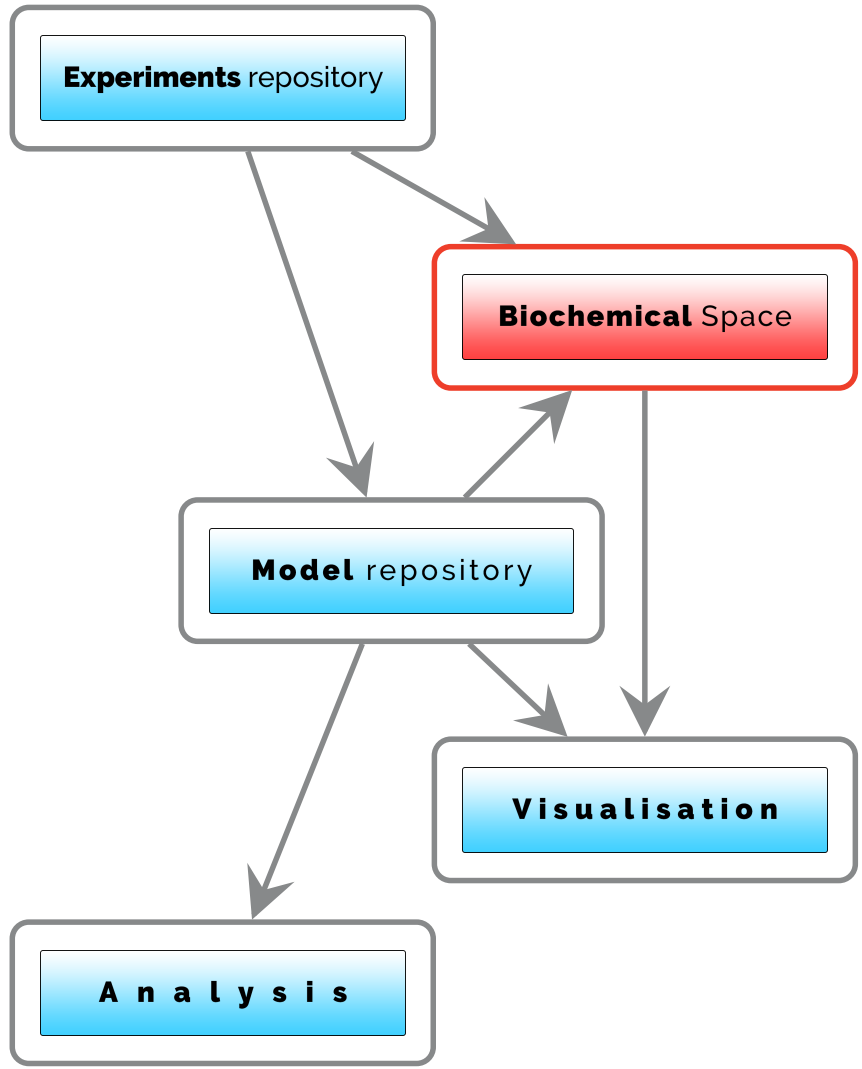
Biochemical Space (BCS)

- rule-based
- acompanied with process hierarchy
- formal description





Biochemical Space (BCS)

Compositional Chemical Entities

Full composition $\rightarrow$ structure of a complex

- KaiBC == KaiC.KaiB
- KaiC6 == KaiC.KaiC.KaiC.KaiC.KaiC.KaiC

Partial composition $\rightarrow$ inner structure of an entity

- KaiC(S{u}|T{p})
- cytb6f(f{-}|bl{n}|bhc{2-})
- ps2(qb{2-}|qa{n}|chl{*}|p680{+}|pheo{-}|oec{4+}|yz{n})

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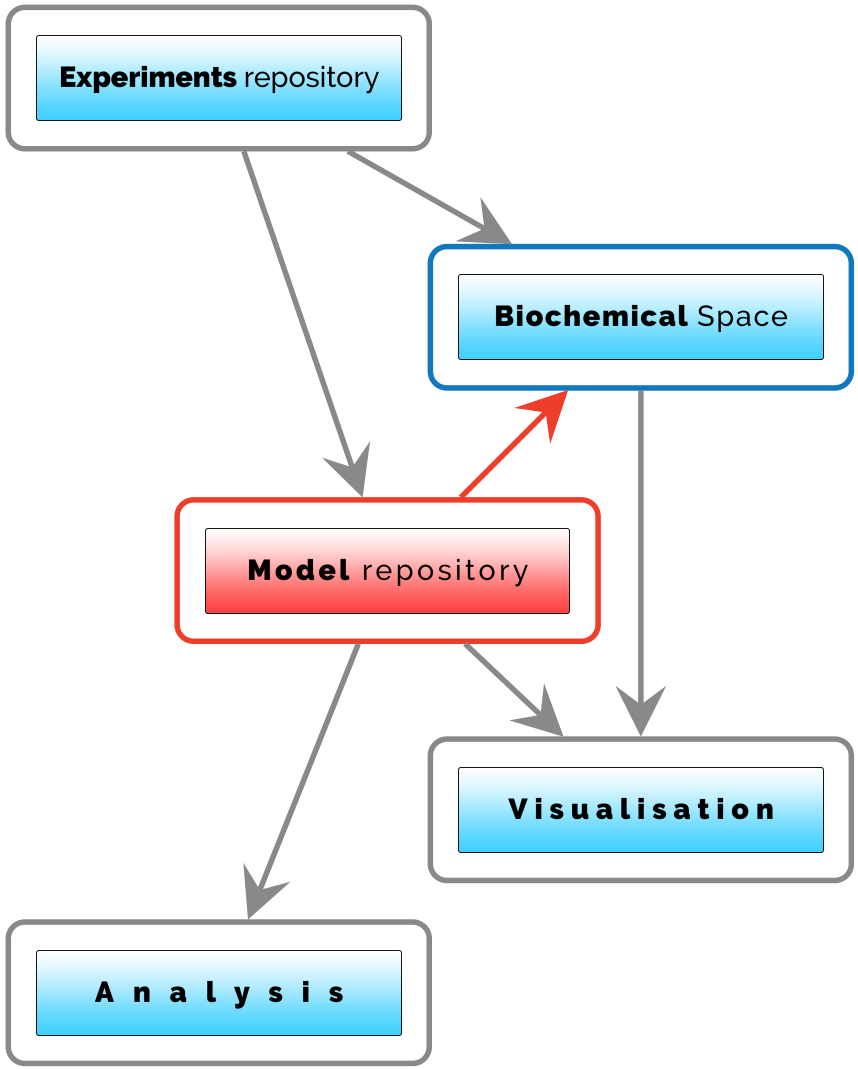
Model repository

- collection of implemented models
- embedded in the process hierarchy
- online simulation with custom parameter settings

→ models are related to BCS which gives them biological sense



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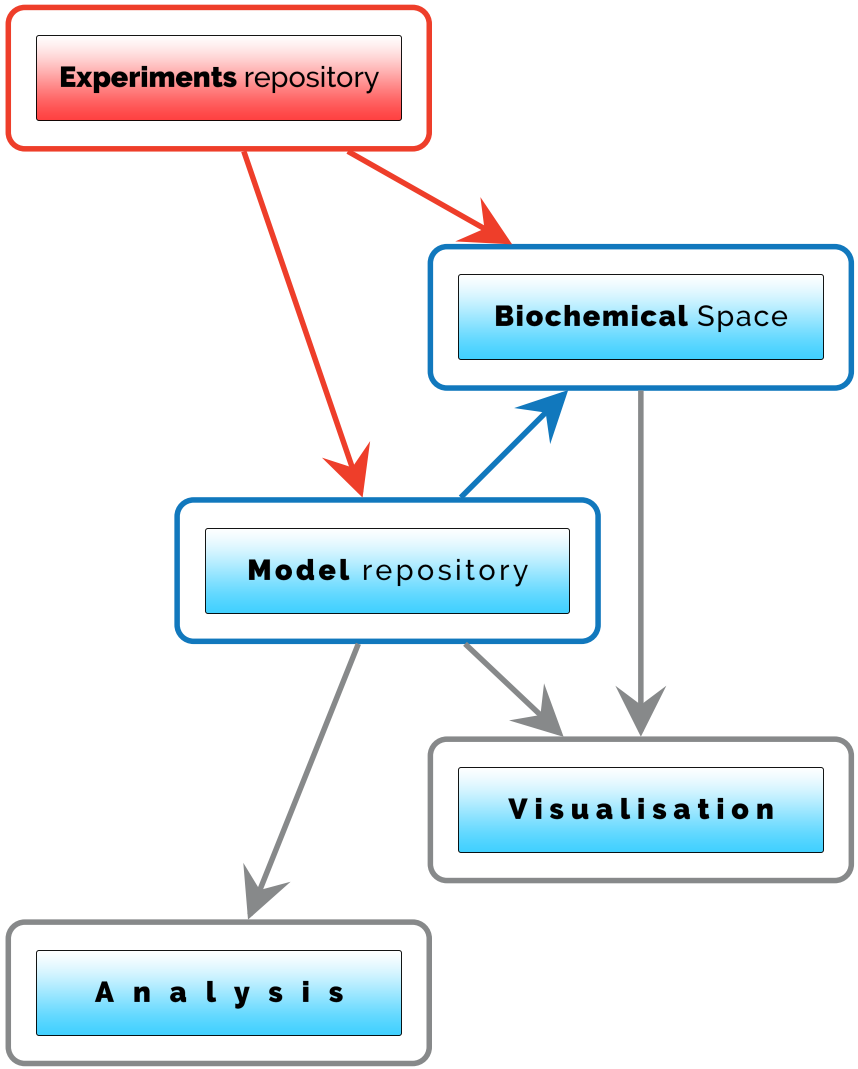
Experiments repository

- storage of time-series data from wet-lab experiments

→ experiments are related to BCS

→ relate an experiment to relevant models



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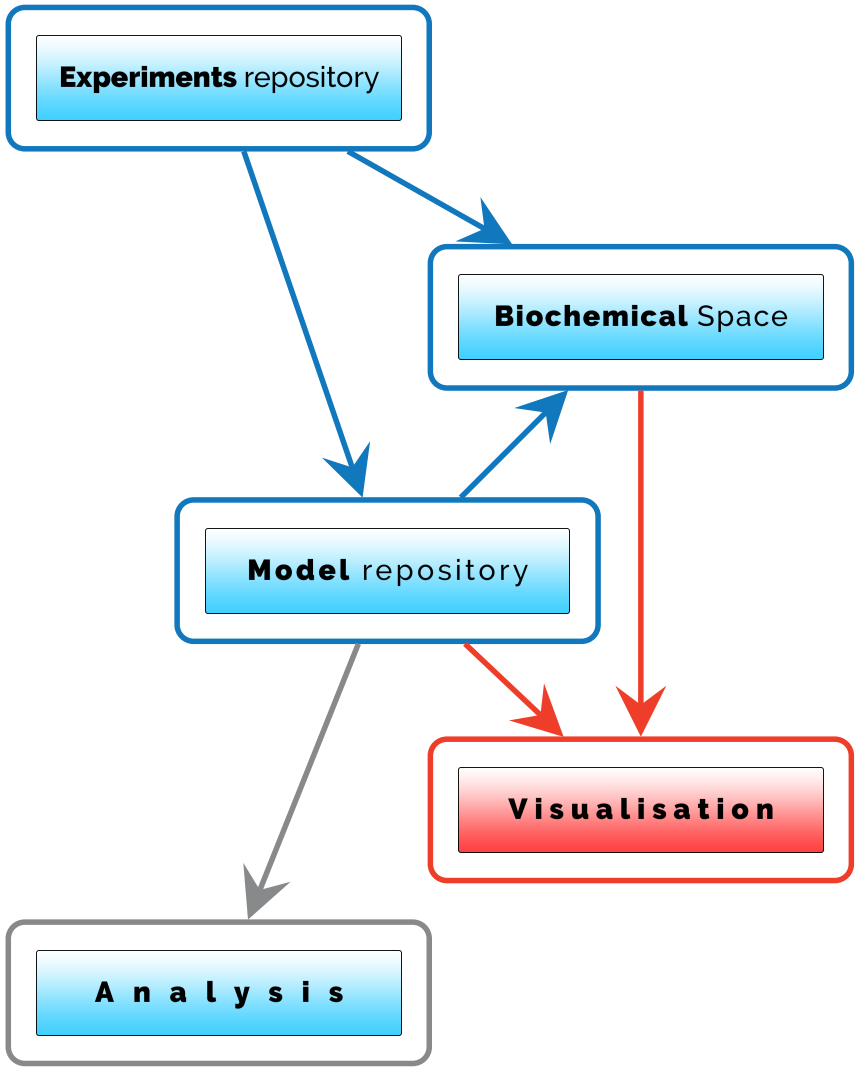
Visualisation

- → static schemes showing particular parts of BCS
- → automatically generated visualisation of reactions/rules
- → simulation charts



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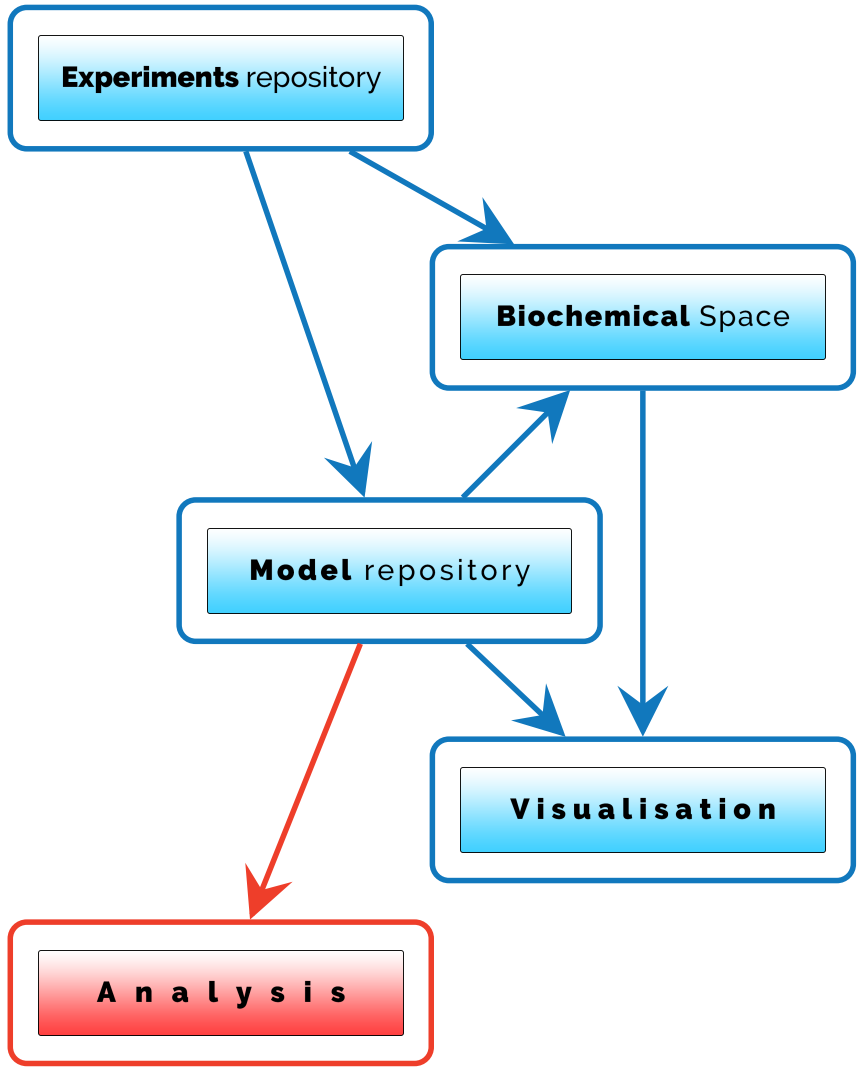
Analysis

→ static analysis of models
- Matrix analysis
- Conservation analysis
- Elementary flux modes analysis



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DEMO

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Future work

- new design
- compartmental hierarchy
- interactive reaction networks visualisation tool
- SBGN visualisation of reaction details
- monitoring and model checking
  $\Rightarrow$ e.g. passing the model to online BioCham
- improve experiment - model relating

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HSB 2016

Fifth International Workshop on Hybrid Systems Biology

Grenoble, France, October 20-21, 2016

Themes

HSB is a systems biology conference series with emphasis on hybrid approaches in a general sense. Hybrid modelling as well as other dynamic modelling approaches are within the scope of the workshop.

Invited speakers

Dennis Bray, University of Cambridge

Albert Goldbeter, Université Libre de Bruxelles

Linda Petzold, University of California

Guillaume Beslon, INSA-Lyon

Program Chairs

Eugenio Cinquemani, INRIA, Grenoble

Alexandre Donzé, University of California

General Chair

Oded Maler, VERIMAG/CNRS, Grenoble

Registration and contacts:
Early bird registration deadline: September 25th

http://hsb2016.imag.fr

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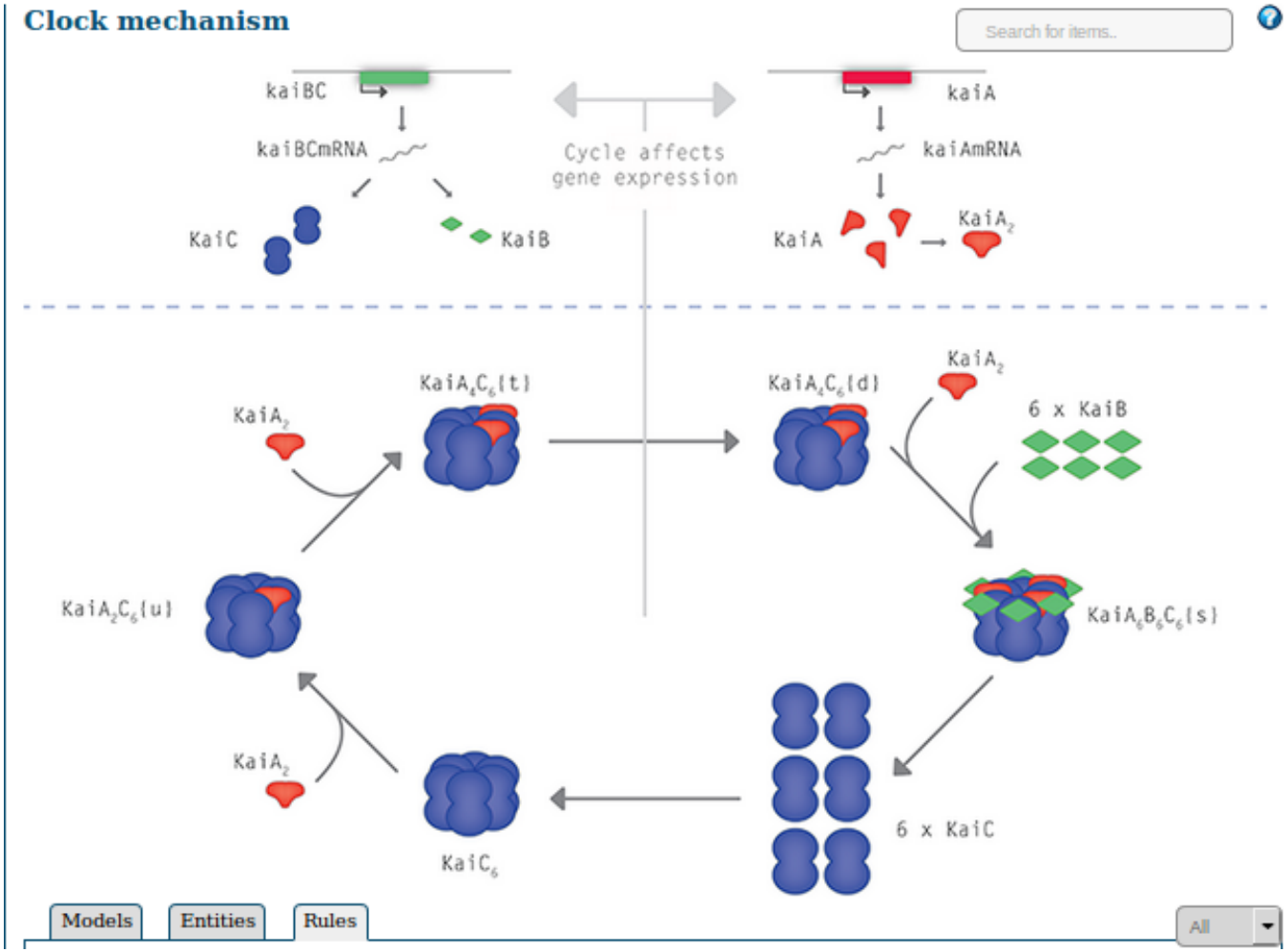
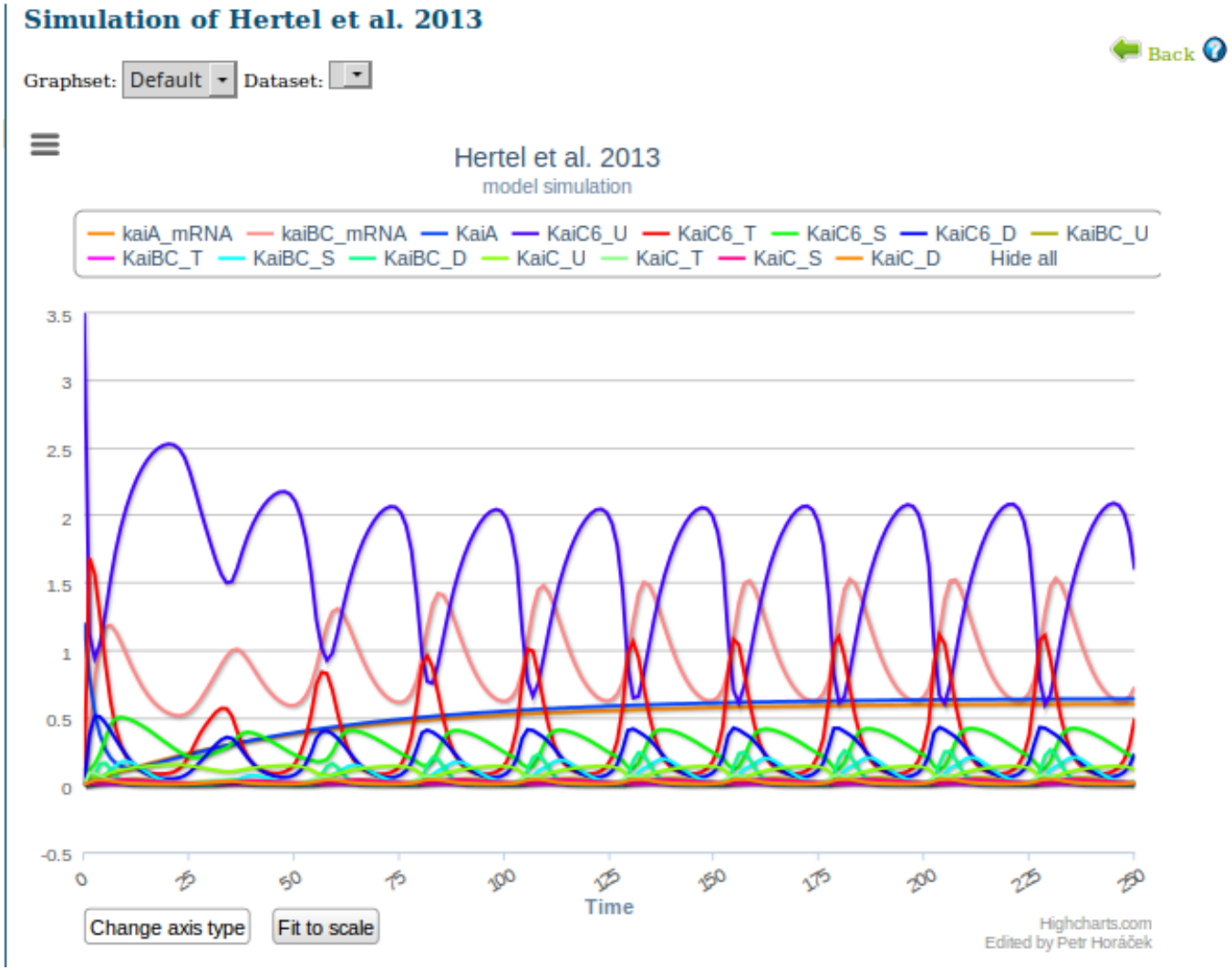
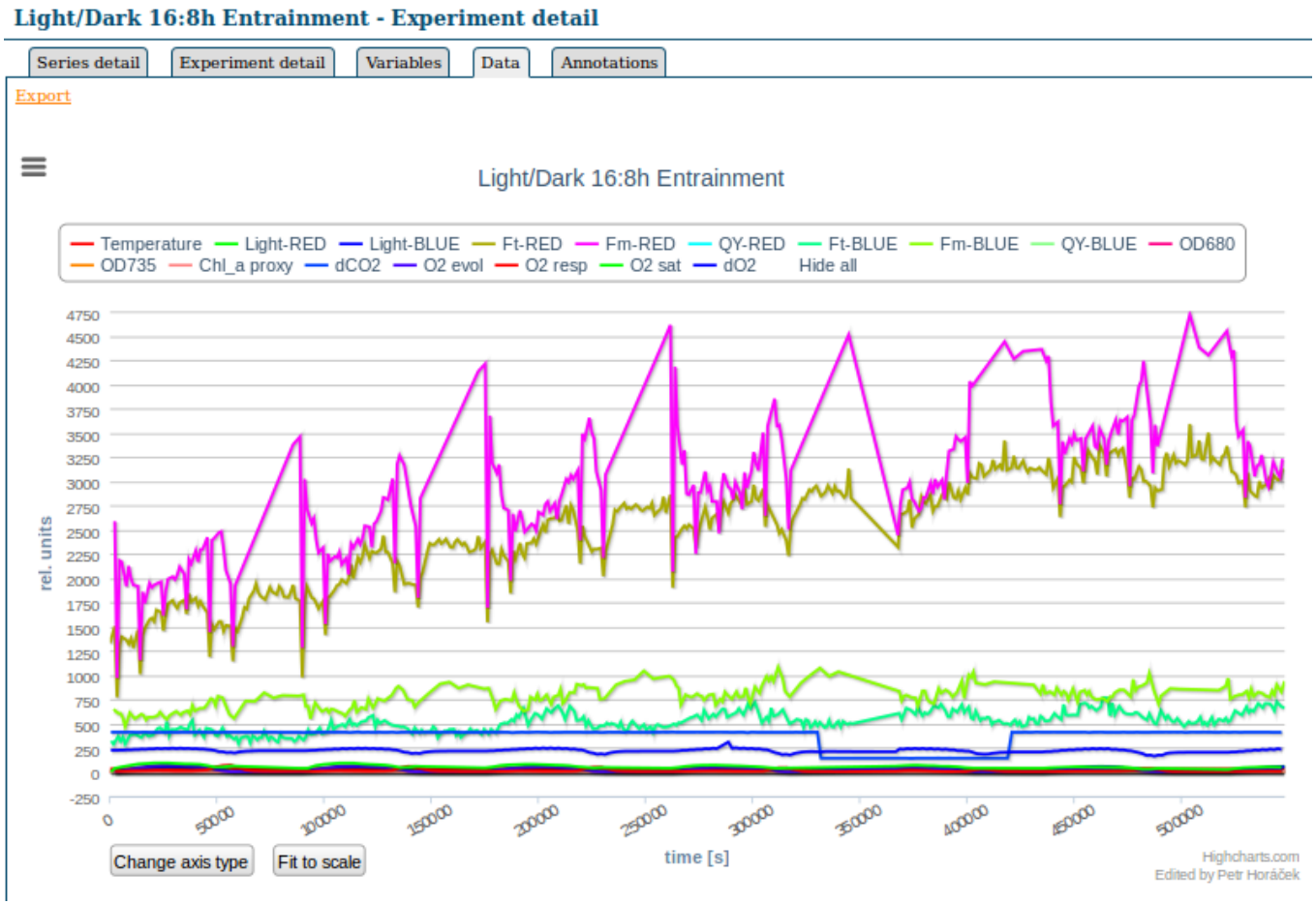
Biochemical Space



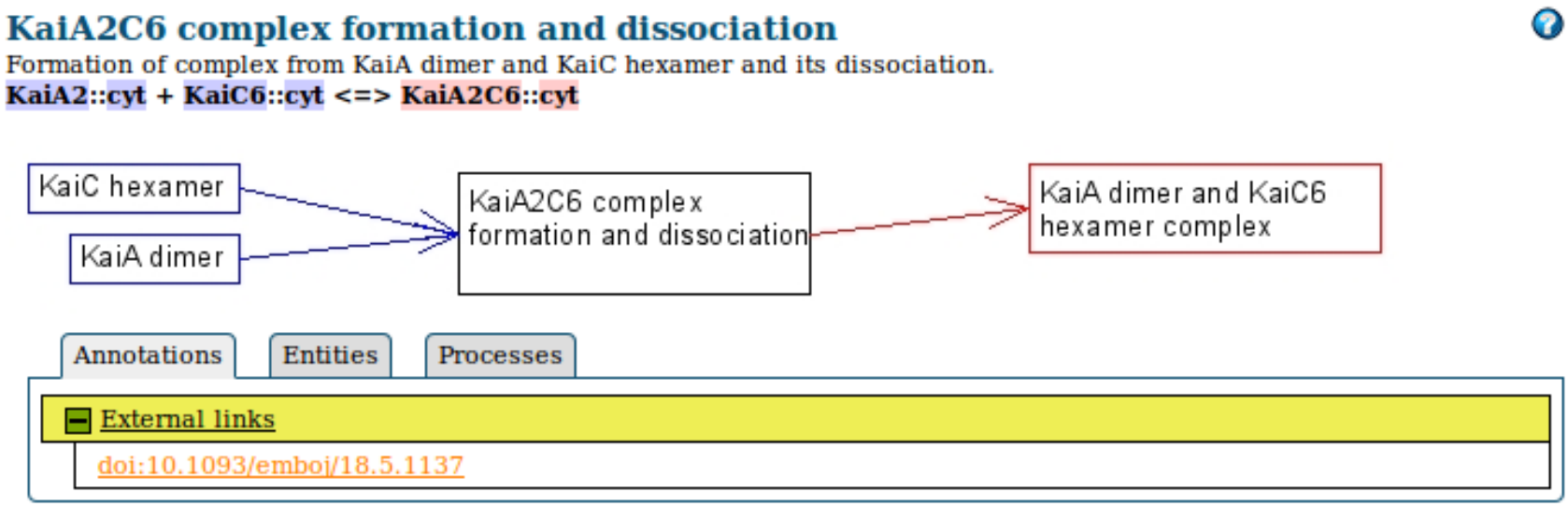
Model repository



Experiments repository



Visualisation



Analysis

Stoichiometry matrix of Müller et al. 2016 (in prep)

	(Rcells_HCO3_m)	(Rcells_CO2)	(RkLa)	(RB)	(RW)	(R2_m)	(R2_p)	(R1_m)	(R1_p)
HCO3_m	1	0	0	0	0	-1	-1	1	1
H_p	0	0	0	1	1	0	1	0	1
dCO2	0	1	1	0	0	0	0	-1	-1
OH_m	0	0	0	0	1	-1	0	-1	0
A_m	0	0	0	1	0	0	0	0	0
CO3_2m	0	0	0	0	0	1	1	0	0
HA	0	0	0	-1	0	0	0	0	0

Analysis data: SBRML

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