

Biochemical Space: A framework for formal description and annotation of complex biological processes

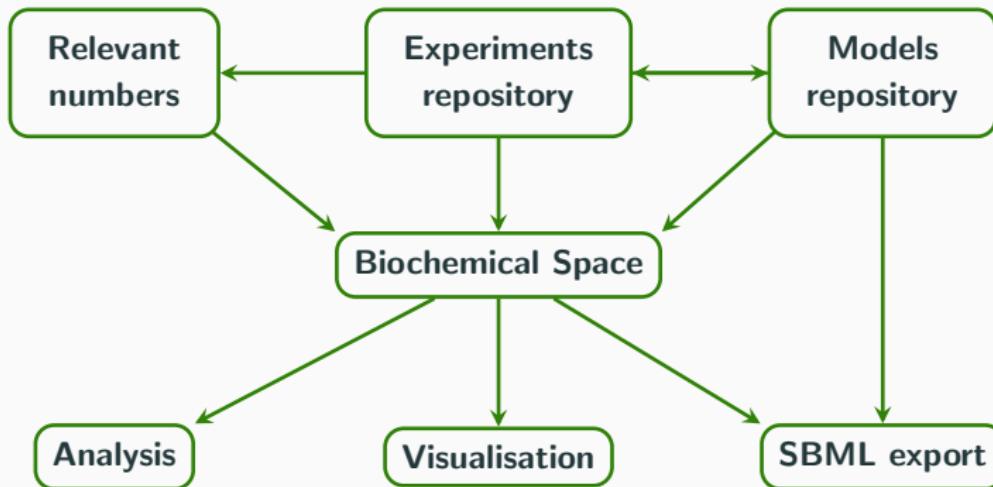
Matej Troják, David Šafránek, Jakub Šalagovič,
Františka Romanovská, and Matej Hajnal

Systems Biology Laboratory @ Masaryk University

Background

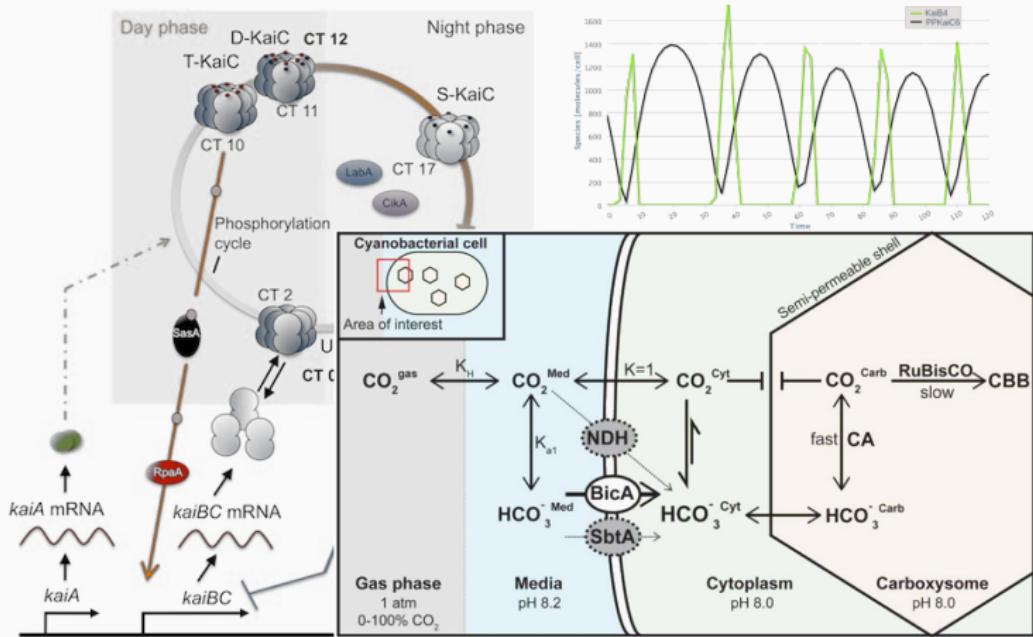
Comprehensive Modeling Platform

Web-based framework for integration of biological knowledge with computational models and wet-lab experiments.



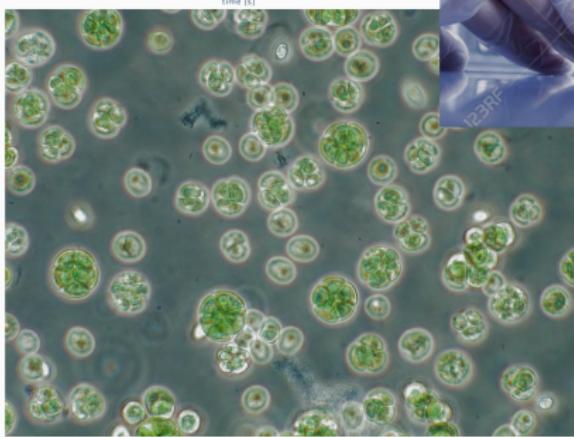
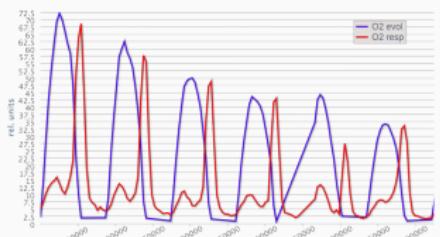
Model repository

- collection of implemented models
- online simulation with custom parameter settings



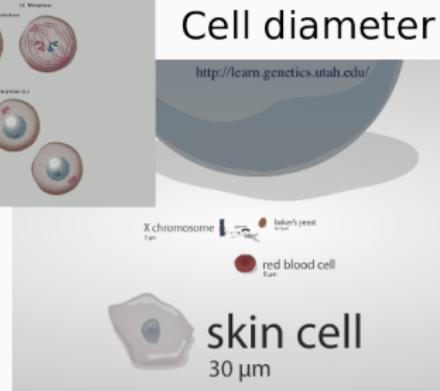
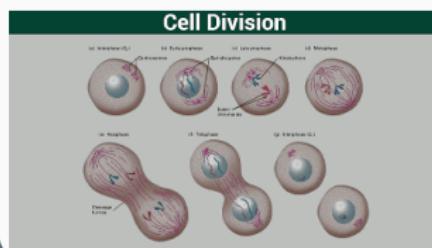
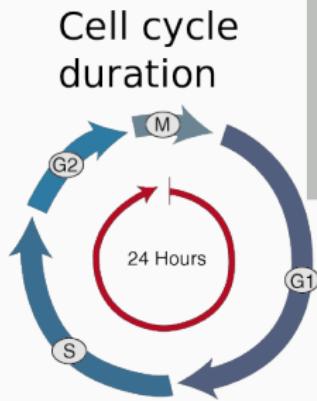
Experiments repository

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



Relevant numbers

- important measured data about biological systems



Annotation

- we can simulate the model – now what?
 - what is biological meaning of the results?
- we have time-series from an experiment – is it confident?
 - what were the conditions?
 - can we repeat the experiment?
- we have a particular value – is it correct?
 - how was it measured?
 - is it organism specific?
- etc.

Biochemical Space (BCS) is a semi-formal knowledge-base providing

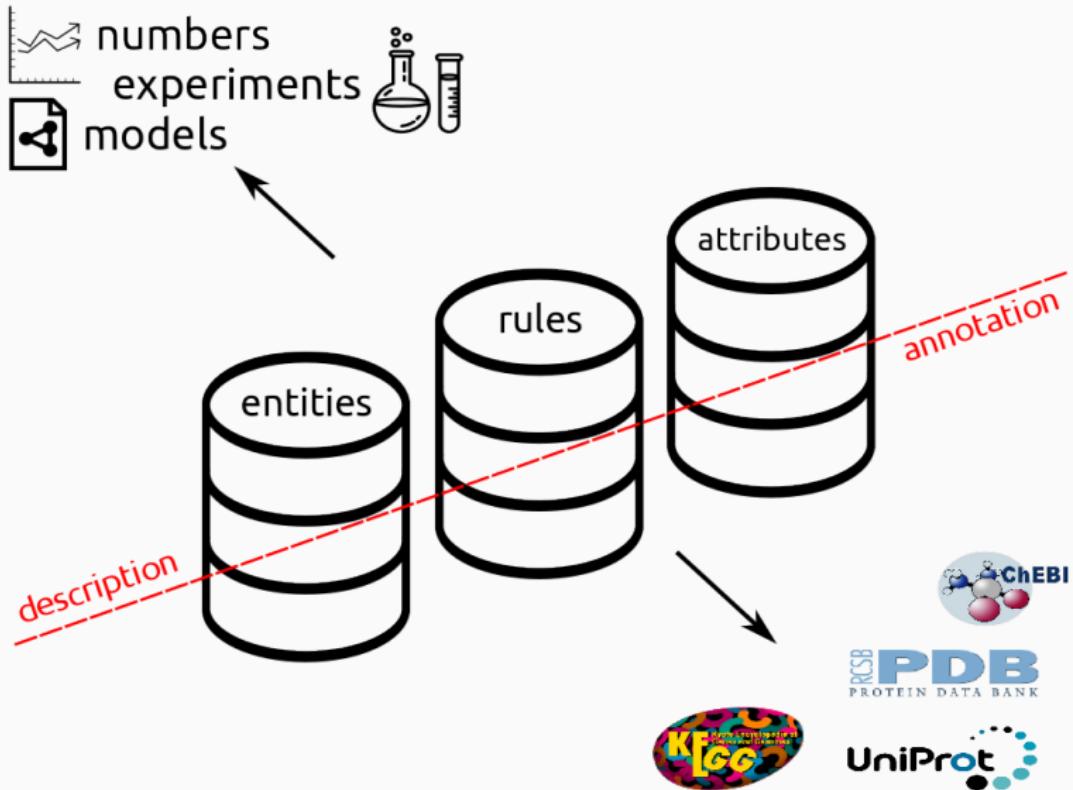
- description,
- annotation,
- public sharing

of domain-specific biological systems.

Formal description of biology preserving relevant **annotation** details.

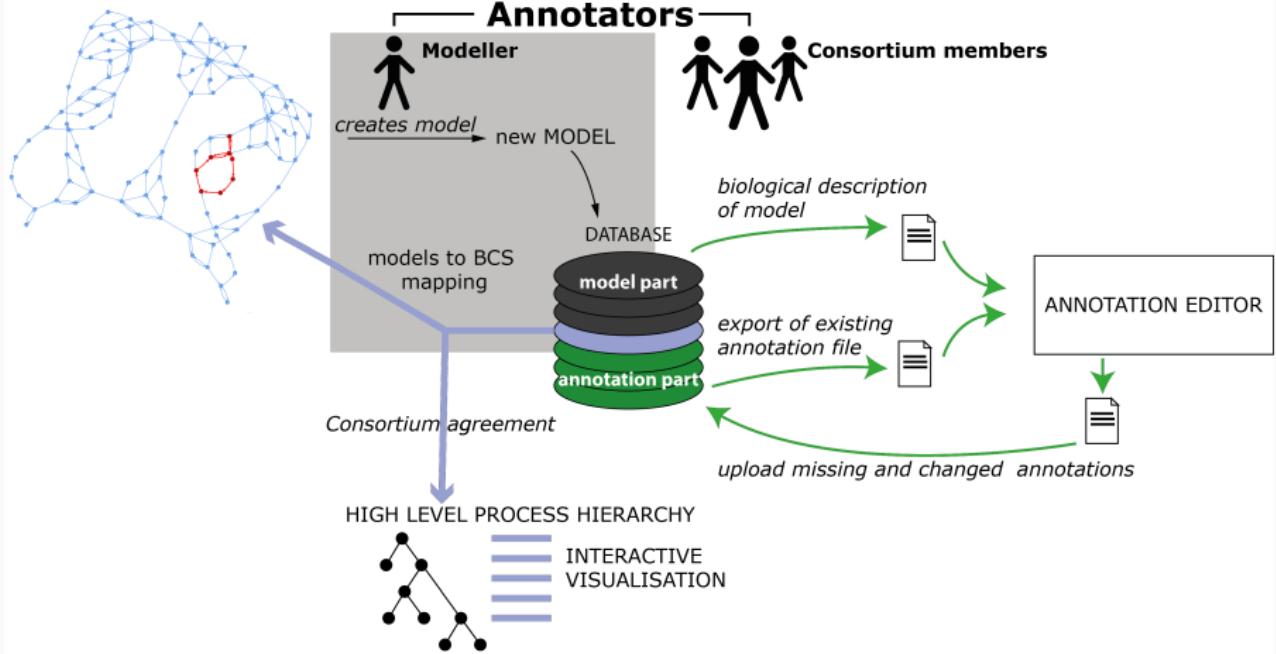
Solves Avoids data re-use problem.

Biochemical Space



- rule-based language – size reduction of entire space
- abstraction of Kappa – neglecting structural features
- direct presentation to the users – *human-readable*
- not just a notation – operational semantics suitable for analysis

How it works



- models
 - relating variables and reactions to BCS (parameters)
 - not necessary 1:1 mapping
 - BCS might be extended (never compressed!)
- experiments
 - relating of variables to BCS
 - particular conditions and equipment
- numbers
 - relating to an attribute and organism/process
 - source (an experiment / **B10NUMB3R5** /...)

Advantages

- gives biological meaning back to the model
 - individual annotation for entities/reactions easily accessible
 - implemented model available online
- BCS for given domain is evolving
 - by each new model, BCS is improved
- helps to reveal differences between models
 - and also what they have in common
- connection between models and experiments (numbers)

Applicability

- range of organisms and processes
- not limited by biology
- e-photosynthesis.org
- e-cyanobacterium.org

E-photosynthesis.org

Home | Introduction | Projects | Links | Team | Contact | Blog | Discussions

Username:
Password:

Light Register Reset password

Projects
Photosynthetic apparatus

Diagram illustrating the Photosynthetic apparatus. It shows the Light Harvesting Complex (LHC) capturing light energy and passing it to the Reaction Center. The Reaction Center consists of the Photosystem II (PSII) and Photosystem I (PSI). PSII uses light energy to split water ($H_2O \rightarrow 2H^+ + O_2$) and produce ATP and $NADPH$. PSII also has a role in the Calvin Cycle. PSII and PSI are connected by electron flow. PSII also provides electrons to PSI. PSI uses light energy to produce ATP and $NADPH$. NADPH and ATP are used in the Calvin Cycle. The Calvin Cycle uses CO_2 and H_2O to produce Glucose.

• e-cyanobacterium.org

E-cyanobacterium.org

Home Biochemical Space Model repository Experiments repository CytosNumbers Support Contact

Username:
Password:

Register Reset password Login

Biological Space

Processes

- Oscillation
- Oscillation in the environment
- Oscillations and metabolism
- Respiration and photosynthesis
- Redox-controlled processes
- Redox-controlled metabolism
- Redox-controlled oscillations
- Redox-controlled metabolism
- Clock mechanism
- Metabolism

Cellular processes

Respiration

Respiration and Photosynthesis

Clock

Metabolism

Transport

Search for terms:

Models | Utilities | Index

• Clark et al. 2014 [in prep]
• Pichard et al. 1995
• Helder et al. 2013
• Dabrowska et al. 2014

Conclusions

Summary

- Biochemical Space as a procedure for annotation of models and other related data

Future work

- SBML-multi package compatibility
- employment of SBGN visualisation
- improvement of:
 - implementation of a new model
 - relating models to BCS
- application on other problems/systems

Acknowledgment



Systems Biology Laboratory

David Šafránek
Jakub Šalagovič
Františka Romanovská
Matej Hajnal

Czech infrastructure for systems biology

c⁴Sys

