

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

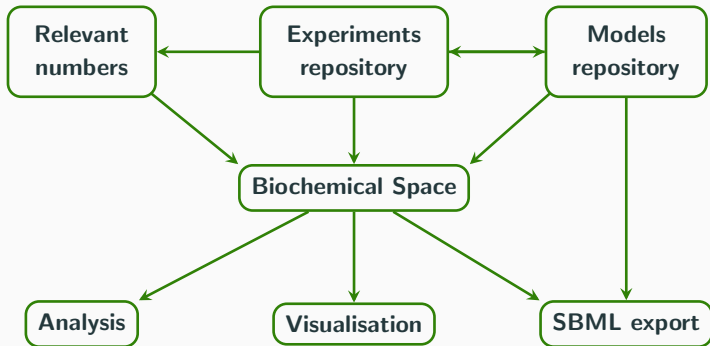
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Matej Troják, David Šafránek, Jakub Šalagovič,  
Františka Romanovská, and Matej Hajnal

Systems Biology Laboratory @ Masaryk University

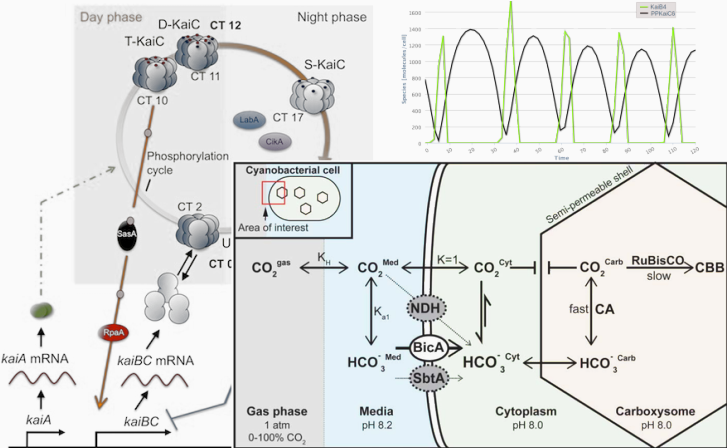
## Comprehensive Modeling Platform

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

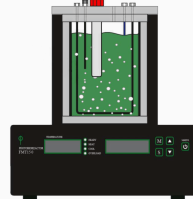
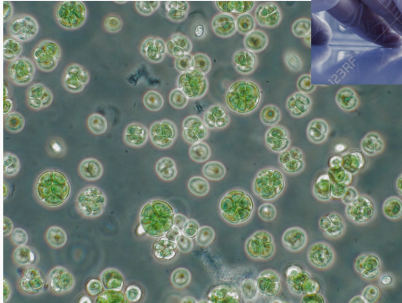
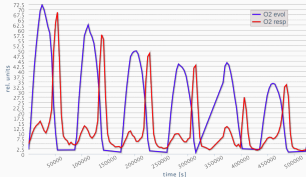


# Model repository

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

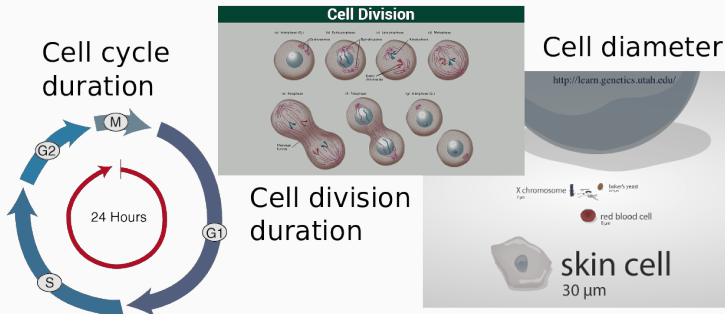


- storage of time-series data from wet-lab experiments



# Relevant numbers

- important measured data about biological systems



- 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

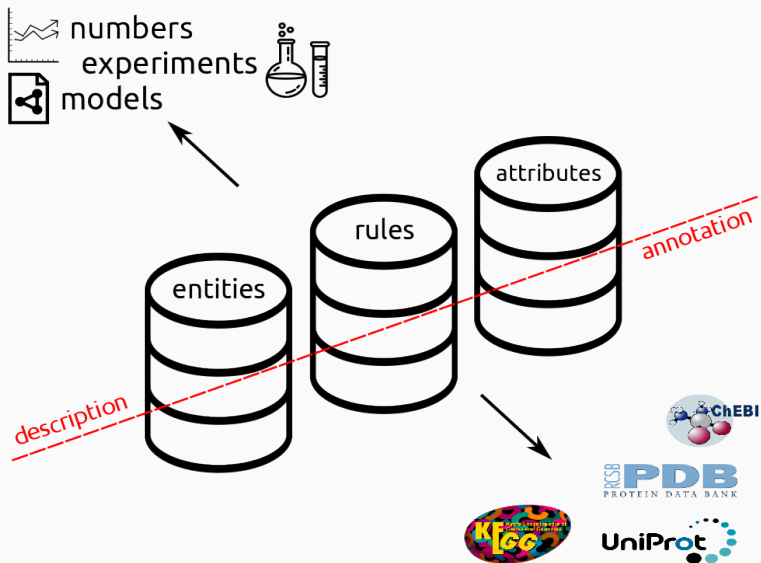
of domain-specific biological systems.

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

Solves Avoids data re-use problem.

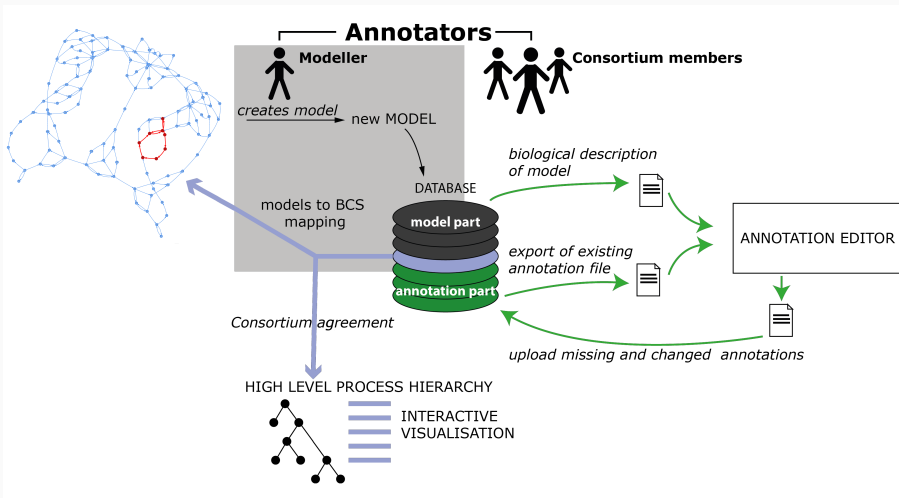
# Biochemical Space





- 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



# 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

The screenshot shows the e-photosynthesis.org website. At the top, there is a navigation bar with links for Home, Introduction, Projects, Links, News, Contact, Blog, and Downloads. Below the navigation bar is a login form with fields for Username and Password, and buttons for Login, Register, and Reset password. The main content area features a 'Projects' section with a list of projects: photosynth\_2009, data\_2002, and data\_2009. The central focus is a diagram titled 'Photosynthetic apparatus' which illustrates the structure of a chloroplast. It shows the 'CALYNEUM HULL' (stroma) containing 'AMYLIC REACTIONS' and 'PHOSPHORYLATION'. The 'THYLAKOID MEMBRANE' is shown with 'LIGHT REACTIONS' occurring there, involving 'PHOTOSYSTEM II', 'PHOTOSYSTEM I', and 'ATP SYNTHASE'. The diagram also labels 'LIPID', 'CHLOROPHYLL', and 'PROTEIN' components.

● e-cyanobacterium.org

The screenshot shows the e-cyanobacterium.org website. At the top, there is a navigation bar with links for Home, Biochemical Space, Model repository, Experiments repository, CyanoNumbers, Support, and Contact. Below the navigation bar is a login form with fields for Username and Password, and buttons for Register, Reset password, and Login. The main content area features a 'Processes' section with a tree view of processes: Environmental processes, Cellular processes, Regulation and homeostasis, Carbon concentration mechanism (CCM), Respiration, Clock, and Metabolism. The central focus is a diagram titled 'Cellular processes' which illustrates the internal structure of a cyanobacterium. It shows 'Respiration' (orange), 'Respiration and Photosynthesis' (green), 'Clock' (blue), 'Metabolism' (purple), and 'Transport' (grey). A red hexagon labeled 'CCH' is also shown. The diagram is set within a cell-like structure with a 'CLOCK' mechanism and 'TRANSPORT' arrows.

## 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



Systems Biology Laboratory

David Šafránek

Jakub Šalagovič

Františka Romanovská

Matej Hajnal

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Czech infrastructure for systems biology

C4Sys

