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

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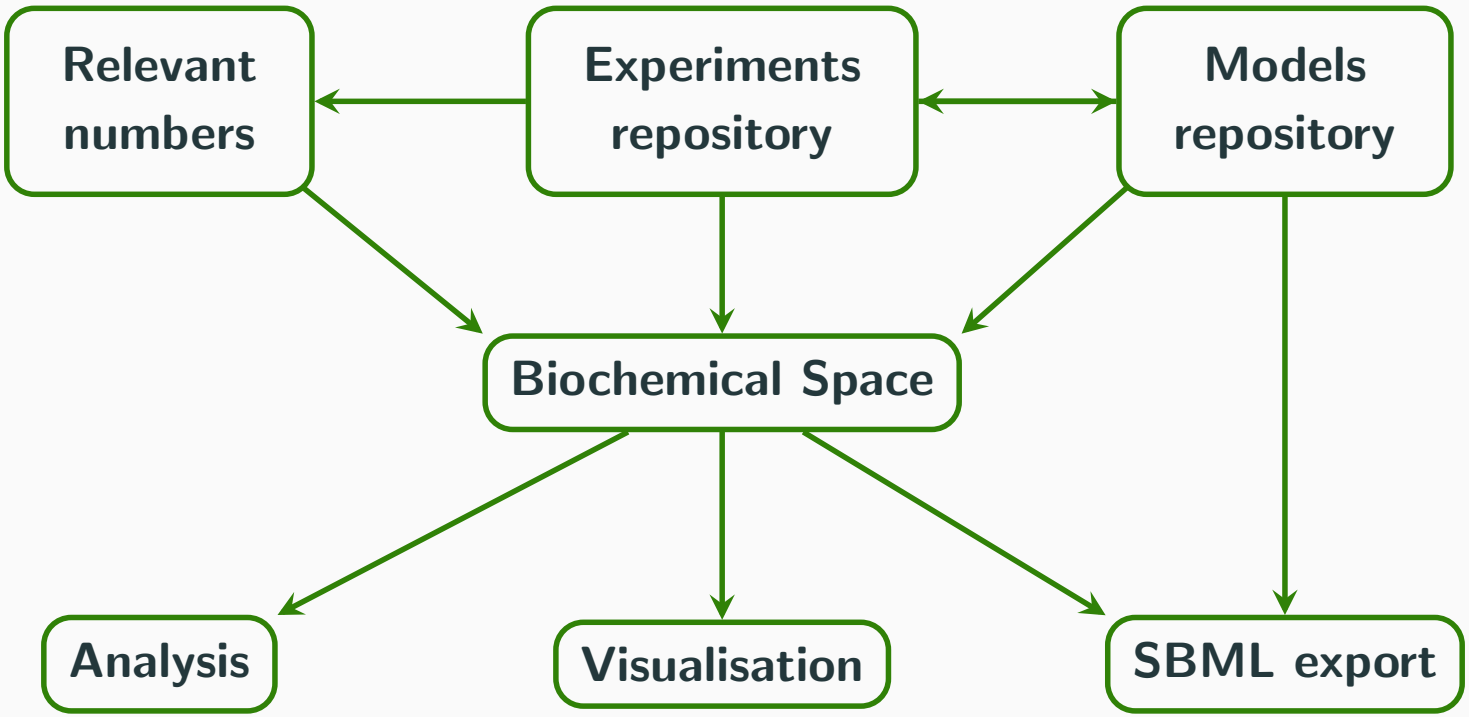
Background

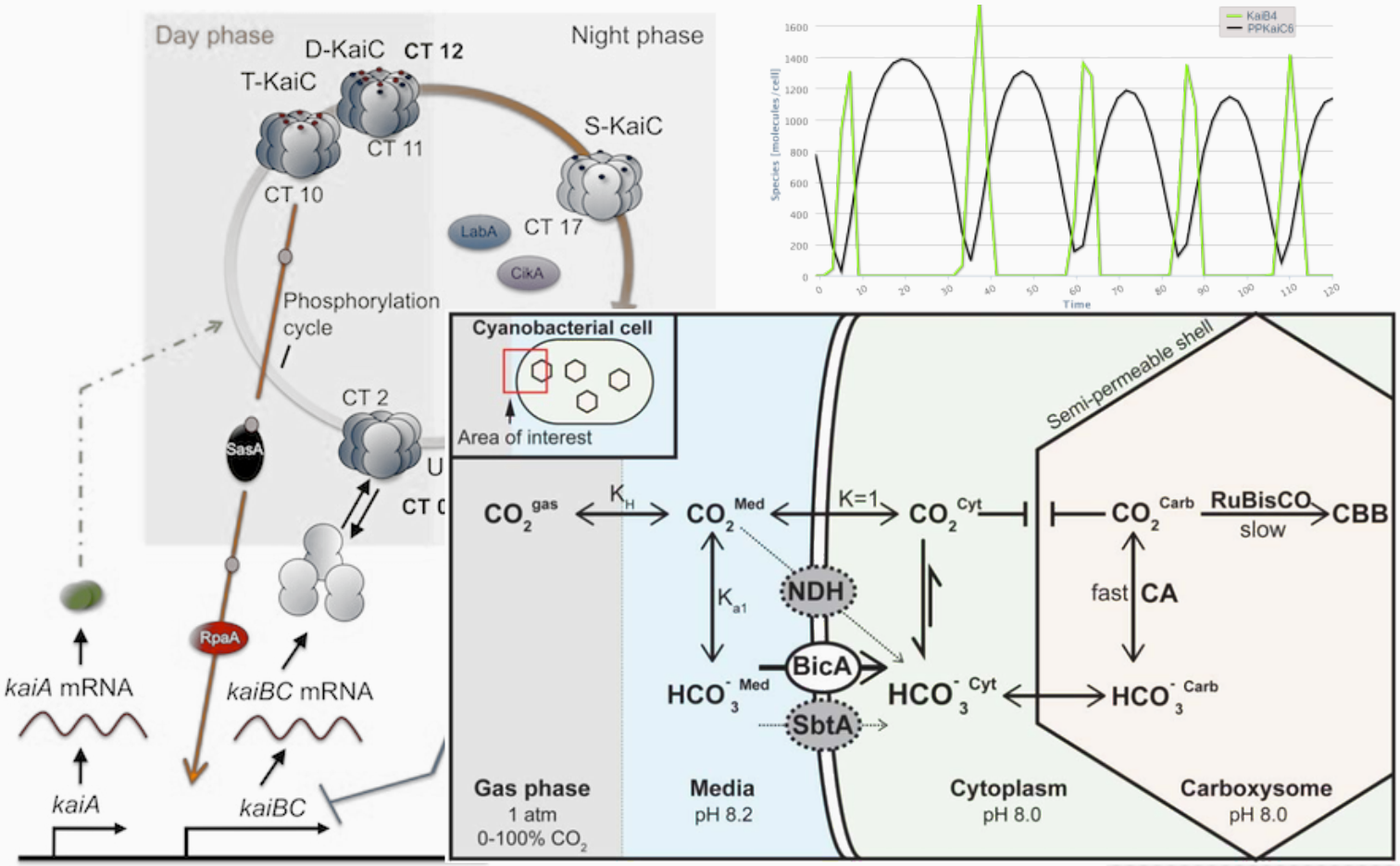
Comprehensive Modeling Platform

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



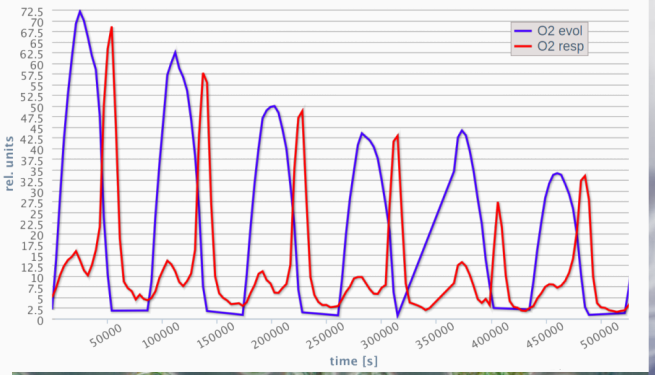
Model repository

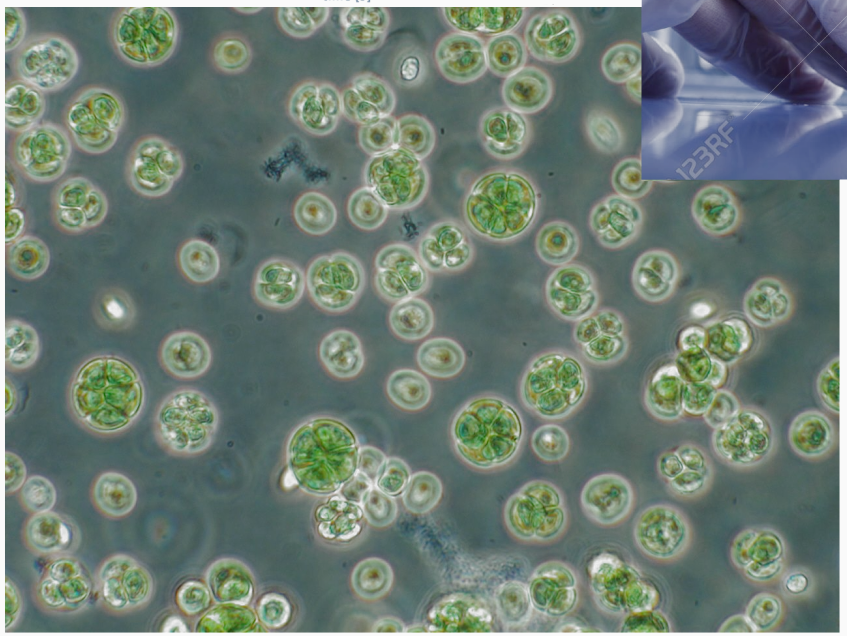
- collection of implemented models
- online simulation with custom parameter settings



Experiments repository

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

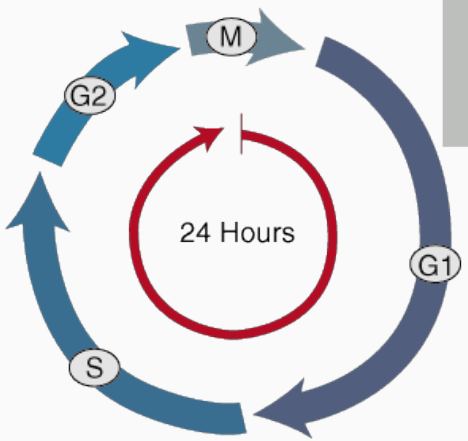


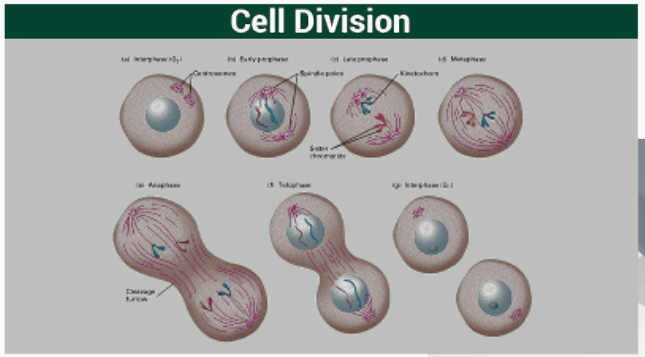


Relevant numbers

- important measured data about biological systems

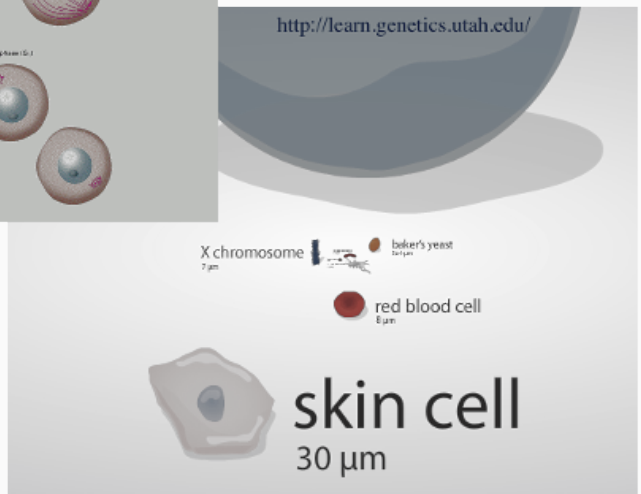
Cell cycle duration





Cell division duration

Cell diameter



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

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

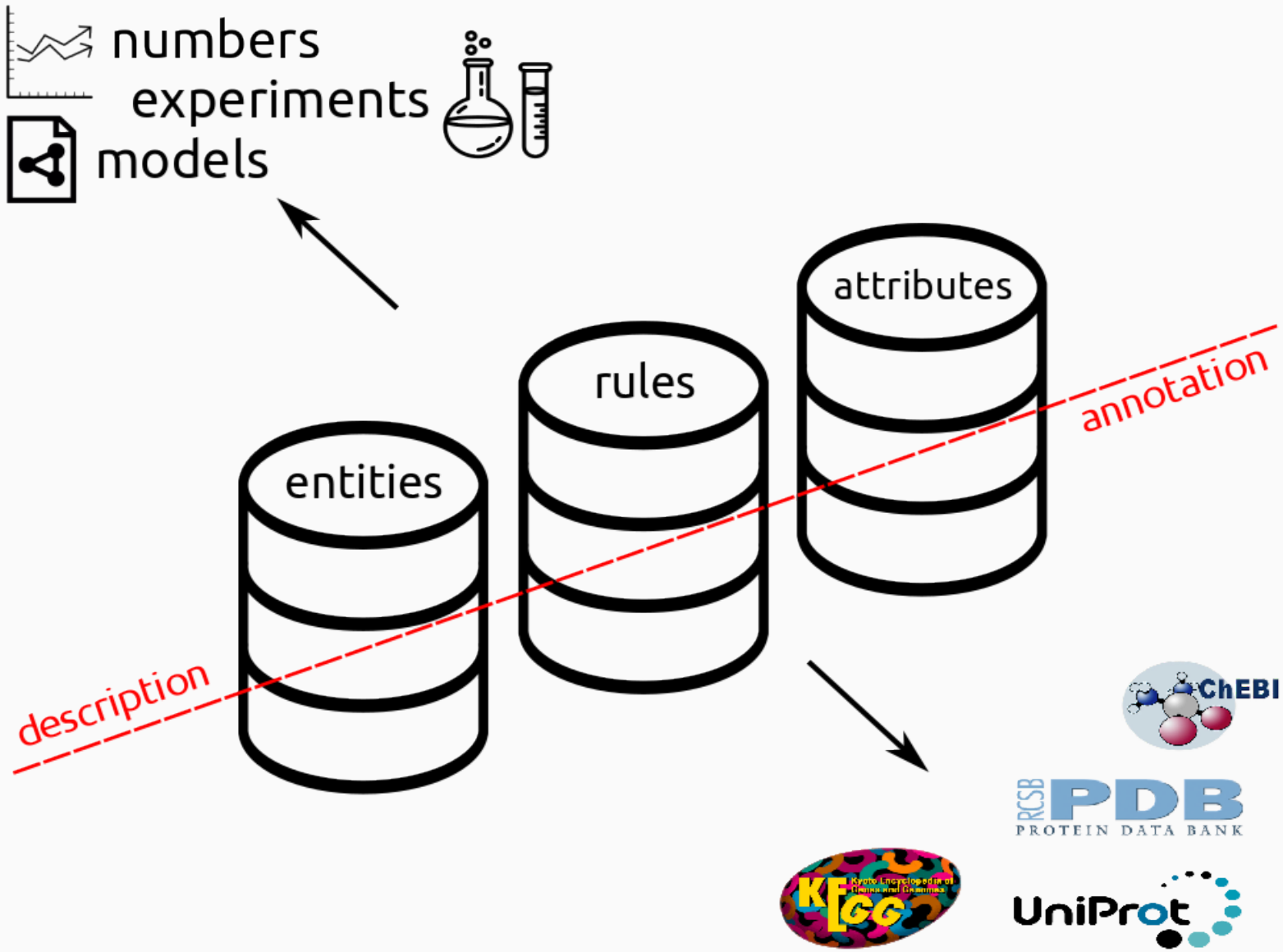
- description,
- annotation,
- public sharing

of domain-specific biological systems.

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

~~Solves~~ Avoids data re-use problem.

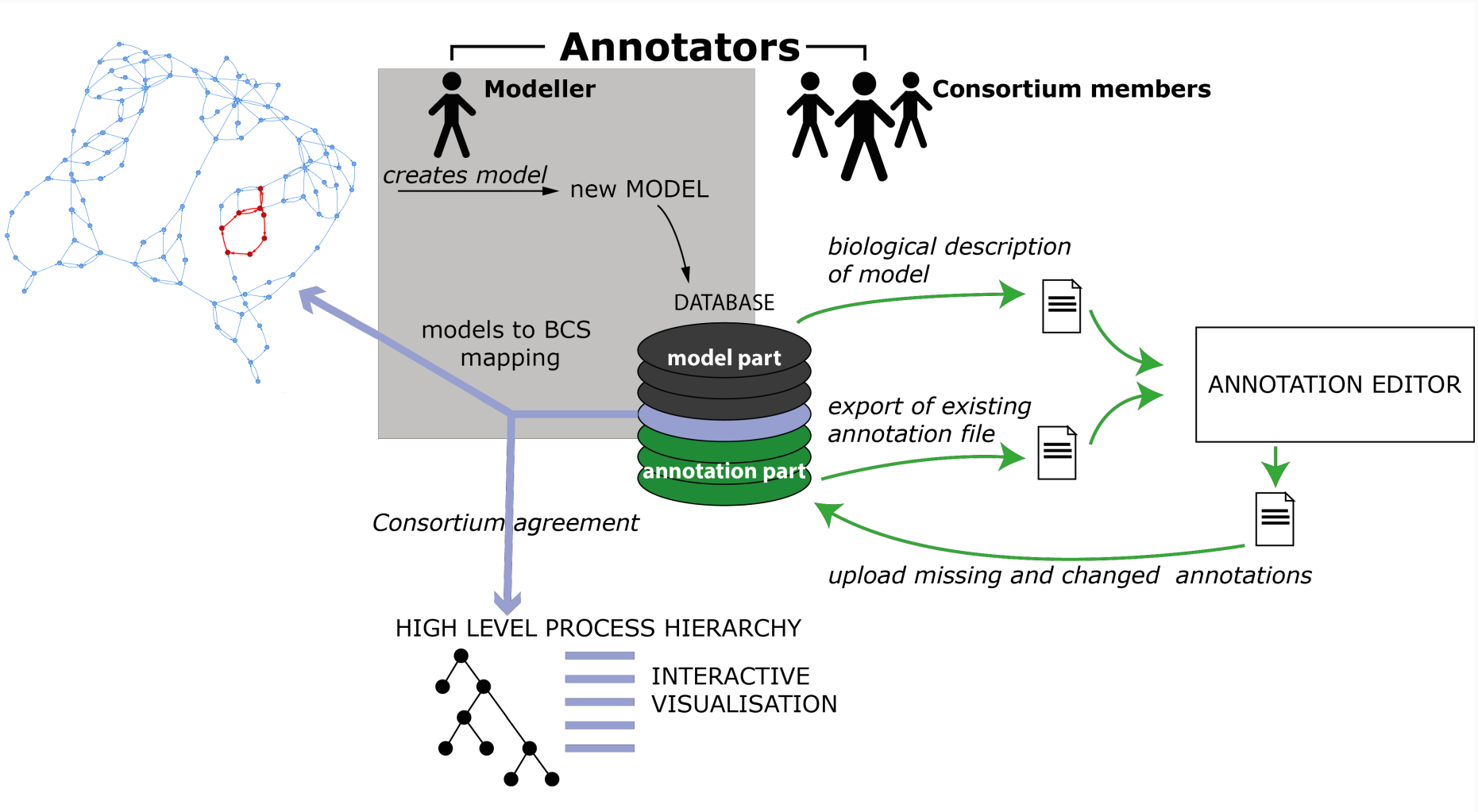
Biochemical Space



Biochemical Space Language

- 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


Annotators
Modeller
Consortium members
creates model
new MODEL
DATABASE
models to BCS mapping
model part
annotation part
biological description of model
export of existing annotation file
ANNOTATION EDITOR
upload missing and changed annotations
Consortium agreement
HIGH LEVEL PROCESS HIERARCHY
INTERACTIVE VISUALISATION

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 / BIONUMB3R5 /...)

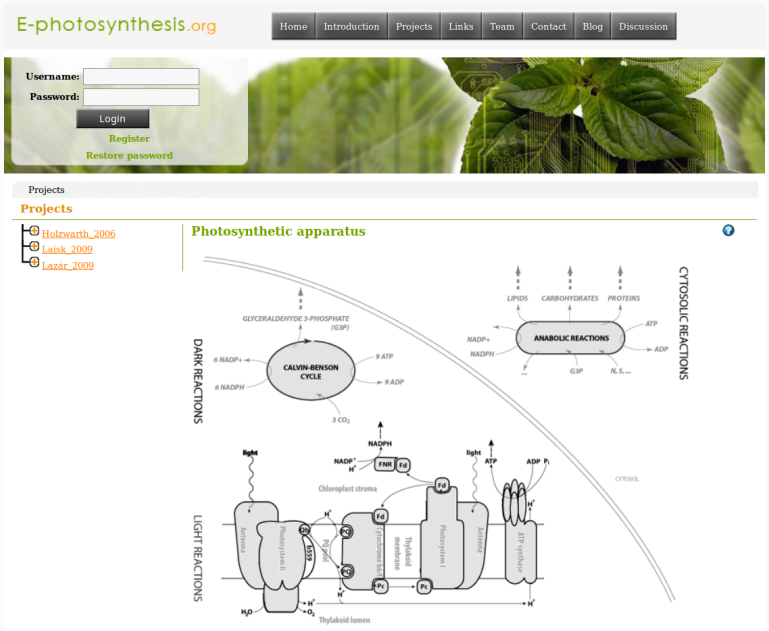
Advantages

- 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)

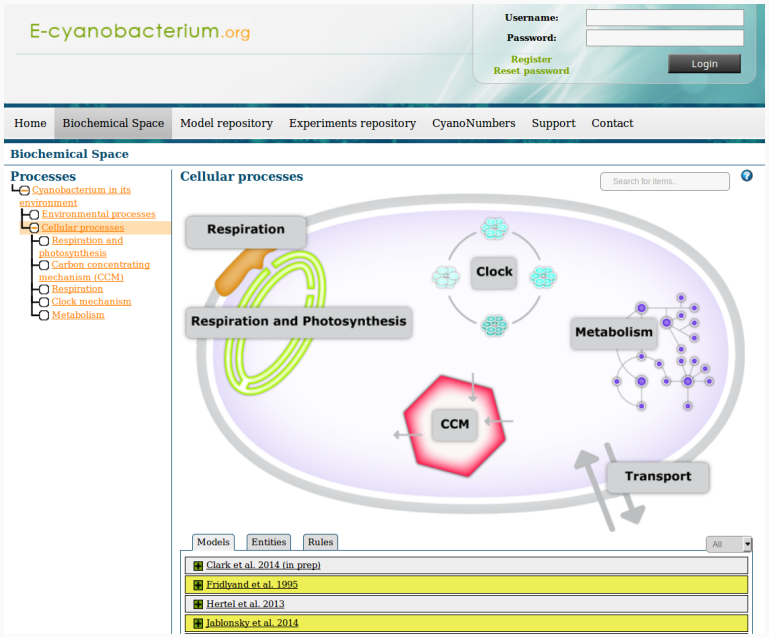
Applicability

- range of organisms and processes
- not limited by biology

- `e-photosynthesis.org`



- `e-cyanobacterium.org`



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

Acknowlegment

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C4Sys