

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

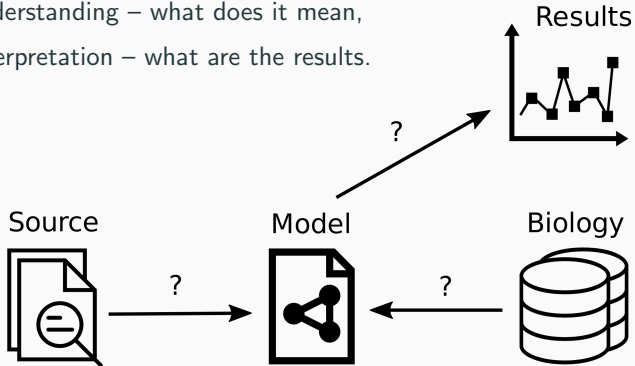
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Motivation

Frequent issues with models:

- reconstruction – get it working,
- understanding – what does it mean,
- interpretation – what are the results.



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

- description,
- annotation,
- public sharing

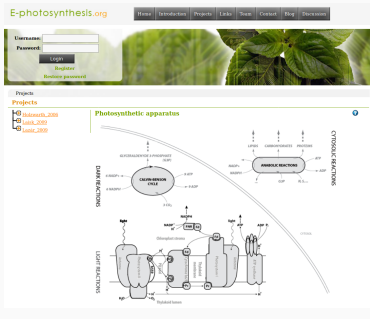
of domain-specific biological models.

Motto: *formalization of biological description while annotating models.*

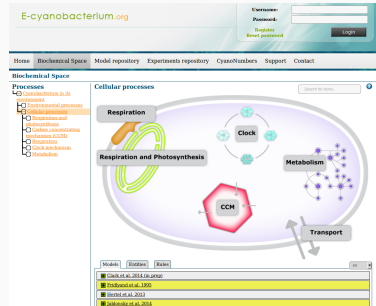
Comprehensive Modeling Platform

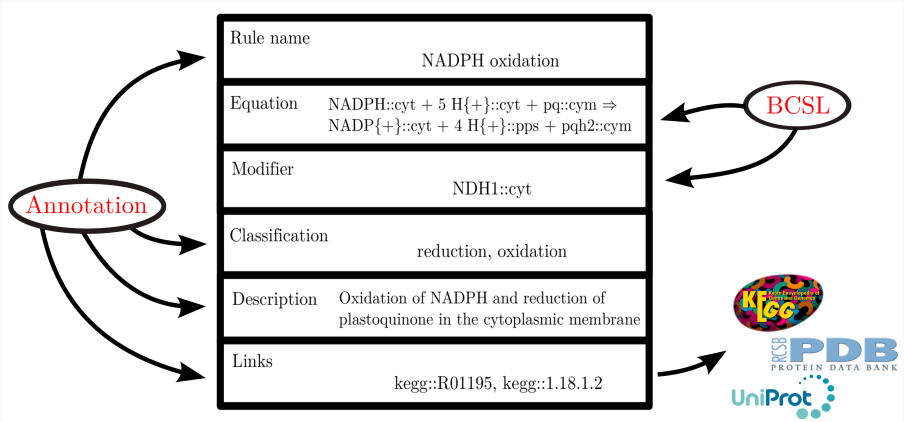
Web-based framework for integration of biological knowledge with computational models and wet-lab experiments.

- e-photosynthesis.org



- e-cyanobacterium.org



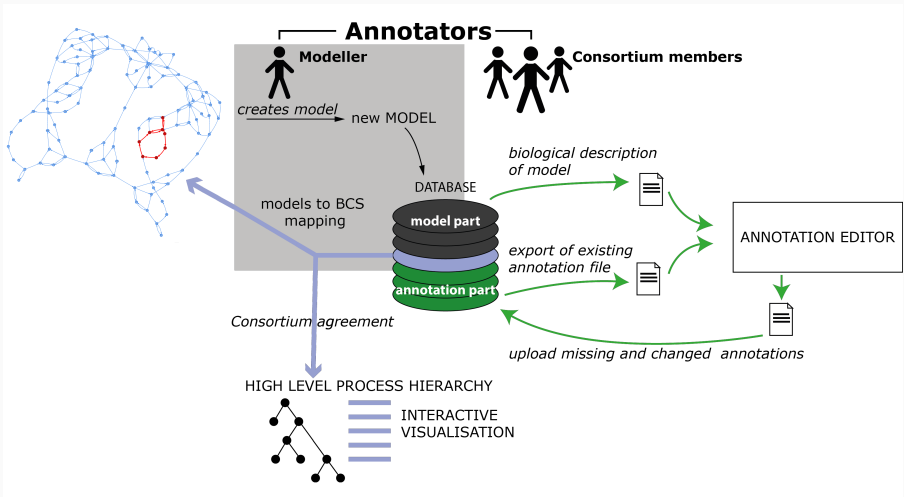


Why new language?

Biochemical Space **Language** (BCSL)

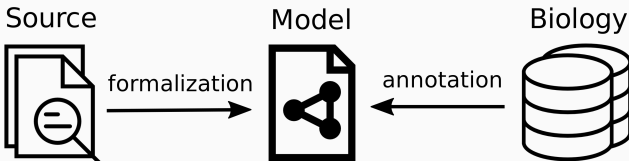
- internal representation easily editable and manageable,
- rule-based – decrease size of the space,
- completely textual – no graphical representation,
- human-readable – direct interpretation to the user,
- not just a notation – operational semantics suitable for analysis (translation to Kappa).

How it works



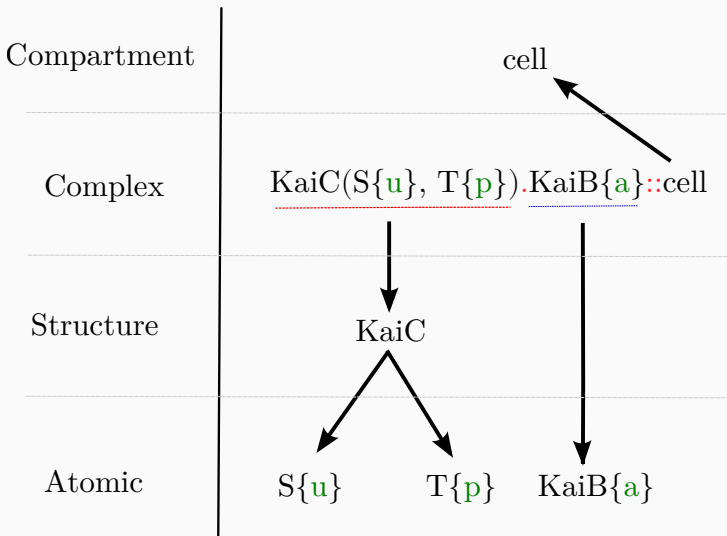
Advantages

- gives the model back its biological meaning
 - individual annotation for entities/reactions easily accessible
 - implemented model available online
- relating to BCS produces model described in BCSL
 - allows further analysis
 - provides qualitative formal description



- helps to reveal differences between models

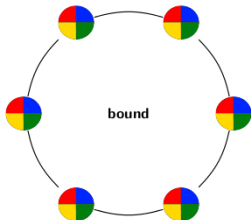
Entities



Abstraction of the complex

Biology

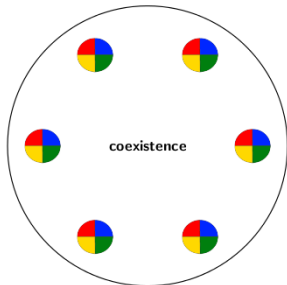
- graph "isomorphism"
- 700 different deviations



- Unphosphorylated protein
- Serine residue phosphorylated protein
- Threonine residue phosphorylated protein
- Both residues phosphorylated protein

BCS abstraction

- mixture $\rightarrow$ order not important
- 84 different deviations



Rules



BCS domain allows further abstractions

Entity ID	KaiC
Entity name	KaiC protein
Composition	S, T
Type	structure
...	

Entity ID	KaiC6
Entity name	KaiC complex
Composition	KaiC.KaiC.KaiC.KaiC.KaiC.KaiC
Type	complex
...	

$$S\{u\}::KaiC::KaiC6::cyt \Rightarrow S\{p\}::KaiC::KaiC6::cyt$$



$$KaiC(S\{u\}).KaiC. \dots .KaiC::cyt \Rightarrow KaiC(S\{p\}).KaiC. \dots .KaiC::cyt$$

Summary

- *Biochemical Space* – framework for process modeling
 - not strictly in the very same configuration
 - usage of alternative representation
-

Future work

- independent operational semantics / improved representation
- custom analysis tool for BCSL models
 - efficient static analysis
- *BCS numbers* extension
 - annotation of parameters