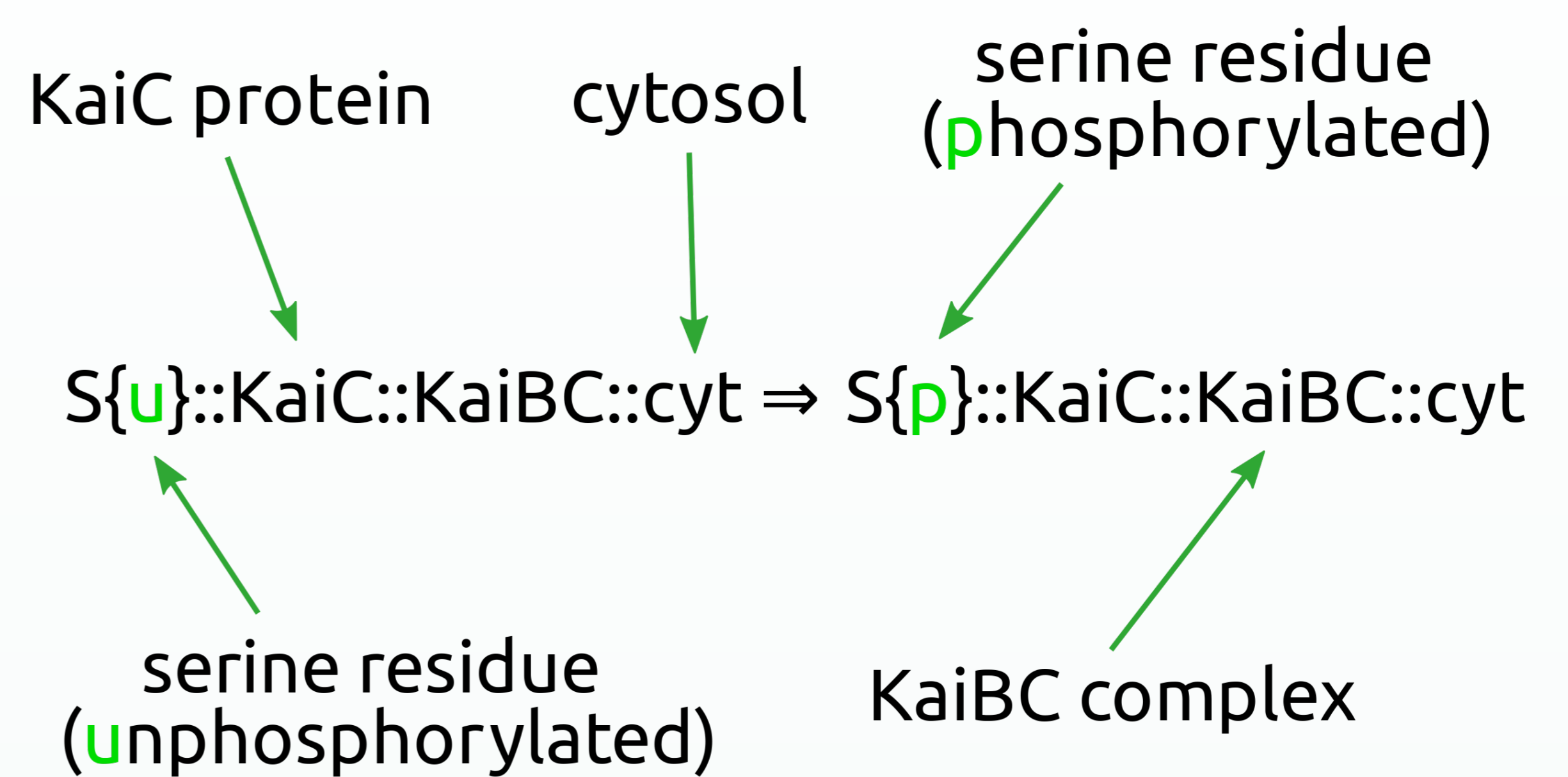


Executable Biochemical Space for Specification and Analysis of Biochemical Systems

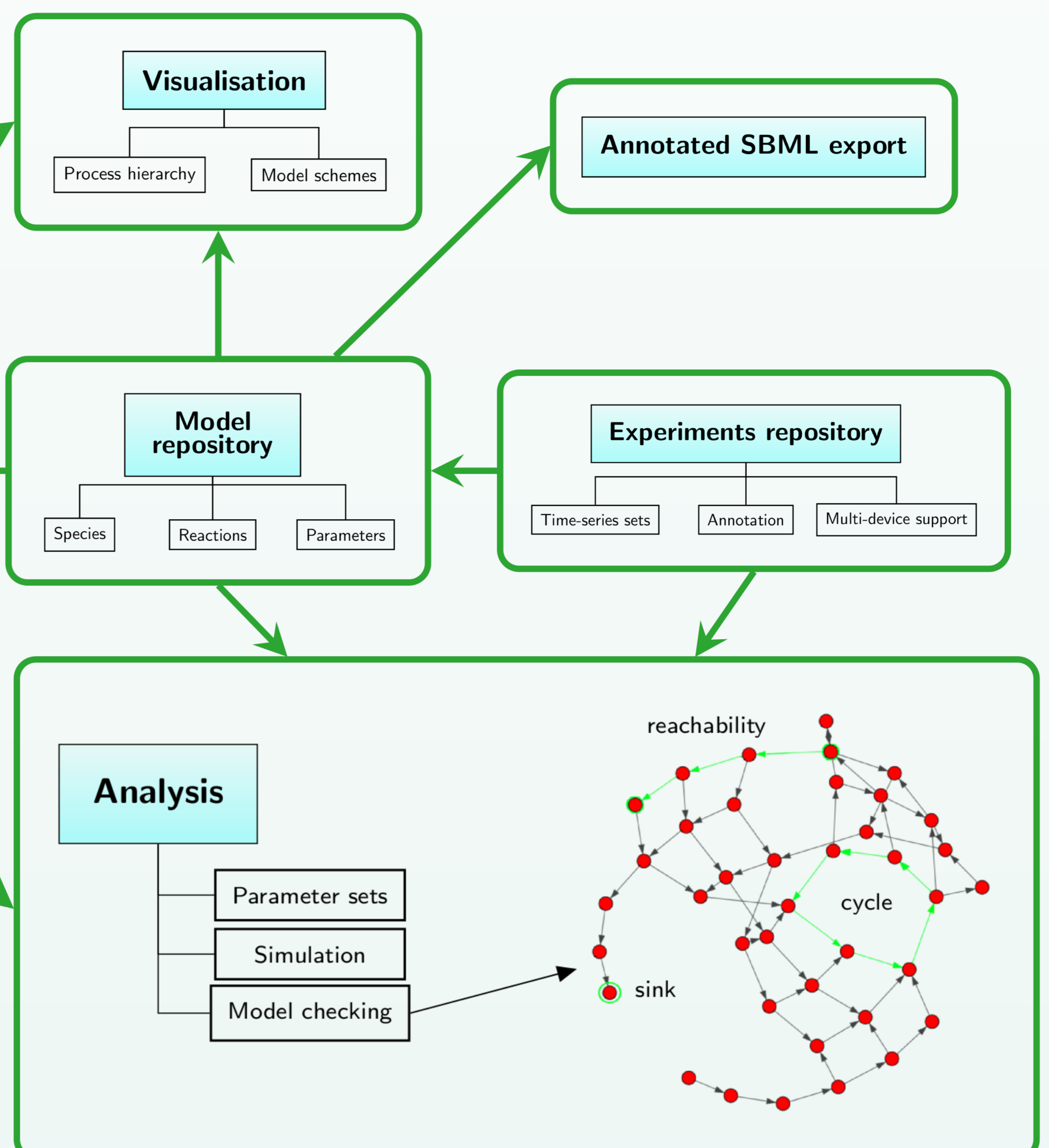
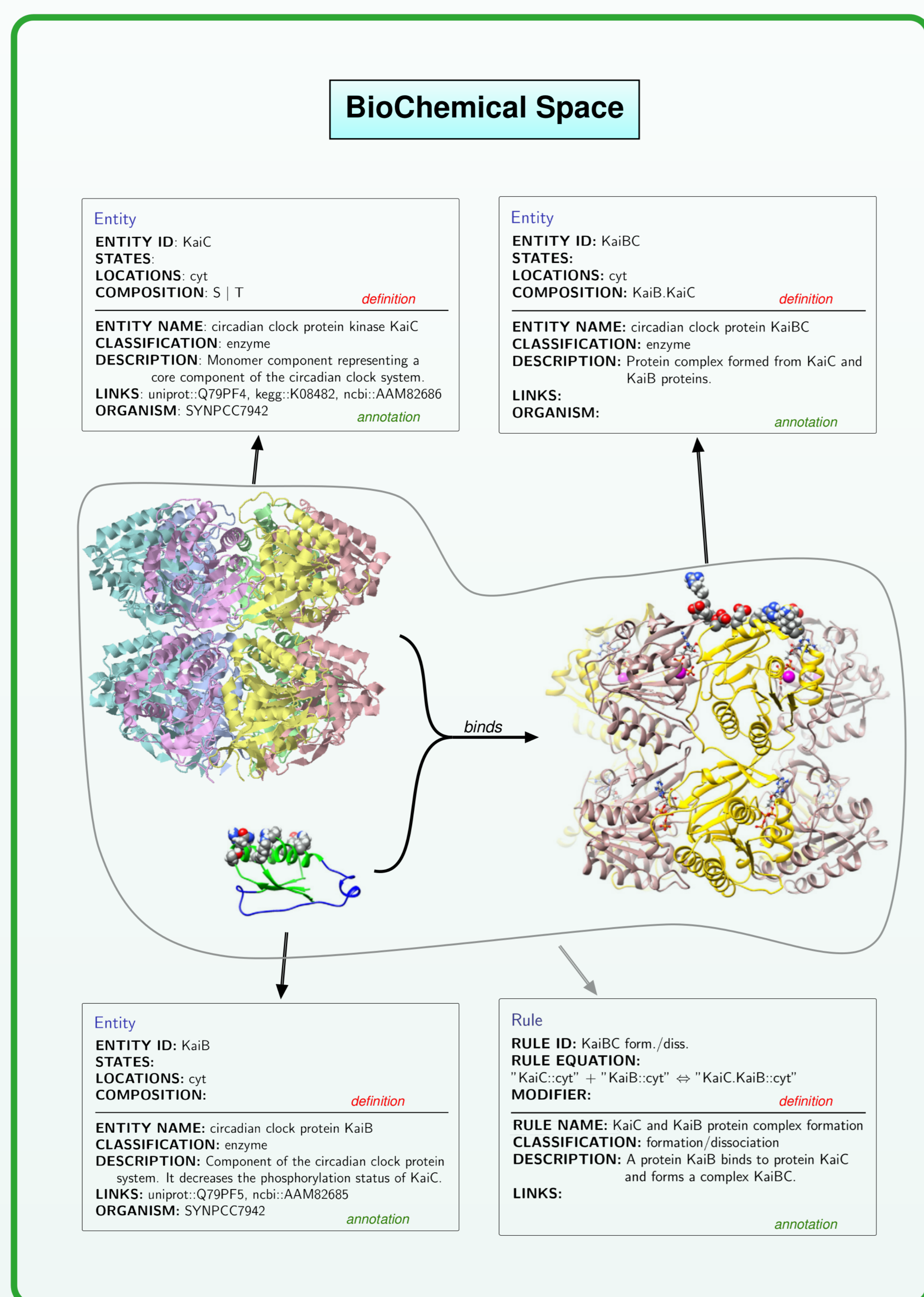
Matej Troják, David Šafránek, Lukrécia Mertová, and Luboš Brim

Biochemical Space (BCS) is a web-based framework for modelling and analysis of biological processes. The concept of BCS forms a crucial part of **Comprehensive Modelling Platform (CMP)** – a general platform for computational modelling and analysis of biological processes. The main goal of BCS is to simplify model-building tasks by providing a simple and clear notation easily understandable by modellers and biologists.

The rigorous core of BCS is called **Biochemical Space Language (BSL)** and is made by declaration of chemical entities and reaction rules. It combines state-of-the-art rule-based techniques with metadata formats developed in well-known annotation databases. The language is formally defined including operational semantics. BCS reflects **SBML level 3** in generalization of compartments in terms of a hierarchy of locations, introducing entity states, and dealing with related combinatorial explosion.



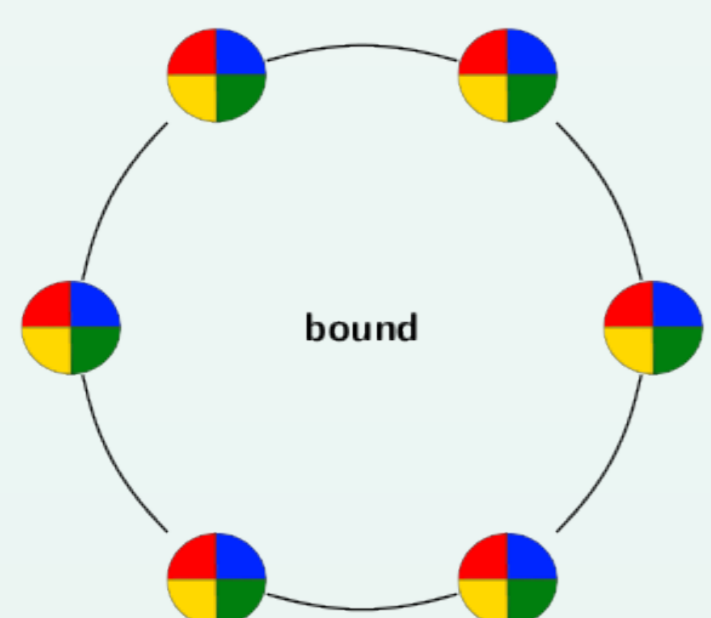
Hierarchical organisation of entities enables zooming into individual parts of composite entities.



Biology

- graph "isomorphism"

- 700 different deviations

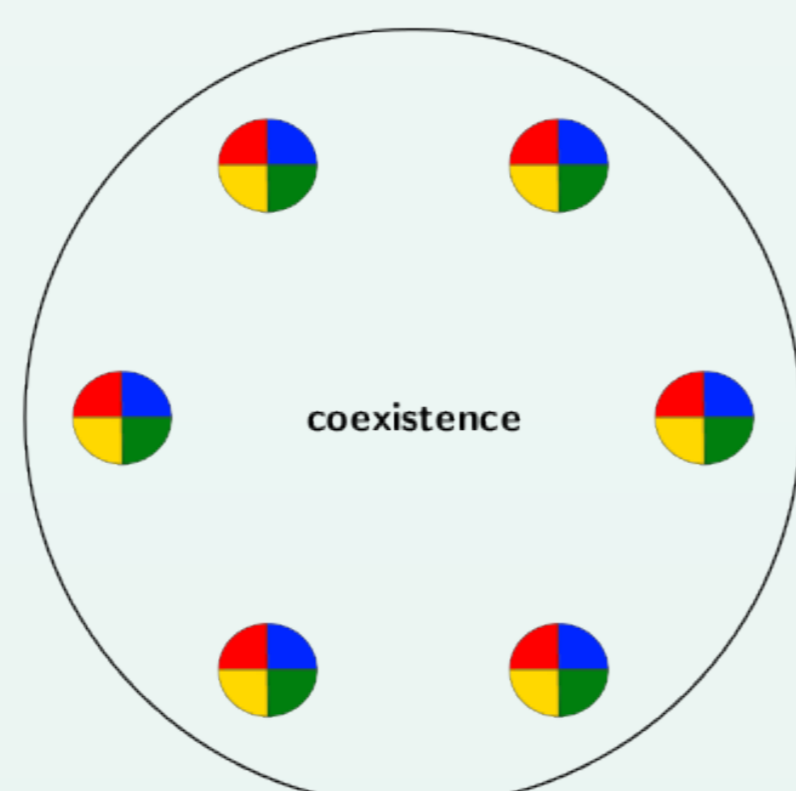


- Unphosphorylated protein
- Serine residue phosphorylated protein
- Threonine residue phosphorylated protein
- Both residues phosphorylated protein

BCS abstraction

- mixture → order not important

- 84 different deviations



BCS abstracts from details of chemical bonds in biochemical complexes. This abstraction significantly decreases number of possible distinguishable entities which can be derived.

The language has the following features:

- description of rules (or reactions) including stoichiometry;
- definition of states encoding different forms of an entity;
- definition of composite entities in an abstract way;
- partial definition of internal entity structure without the need to enumerate all possibilities (e.g., a serine-phosphorylated protein);
- spatial organisation of entities in terms of hierarchical locations;
- variables minimising the need for repetitive definitions of similar objects.

An example of existing application of BCS is available at e-cyanobacterium.org, a web-based platform for the modelling and analysis of biological processes occurring in cyanobacteria. The platform provides several features that contribute to the production and presentation of models targeting cyanobacteria. The principal effort is to interlink the biological knowledge of cyanobacteria with the benefits of computational systems biology tools. The following processes of cyanobacteria are covered: environmental processes, respiration and photosynthesis, carbon concentrating mechanism, circadian clock, and metabolism.