

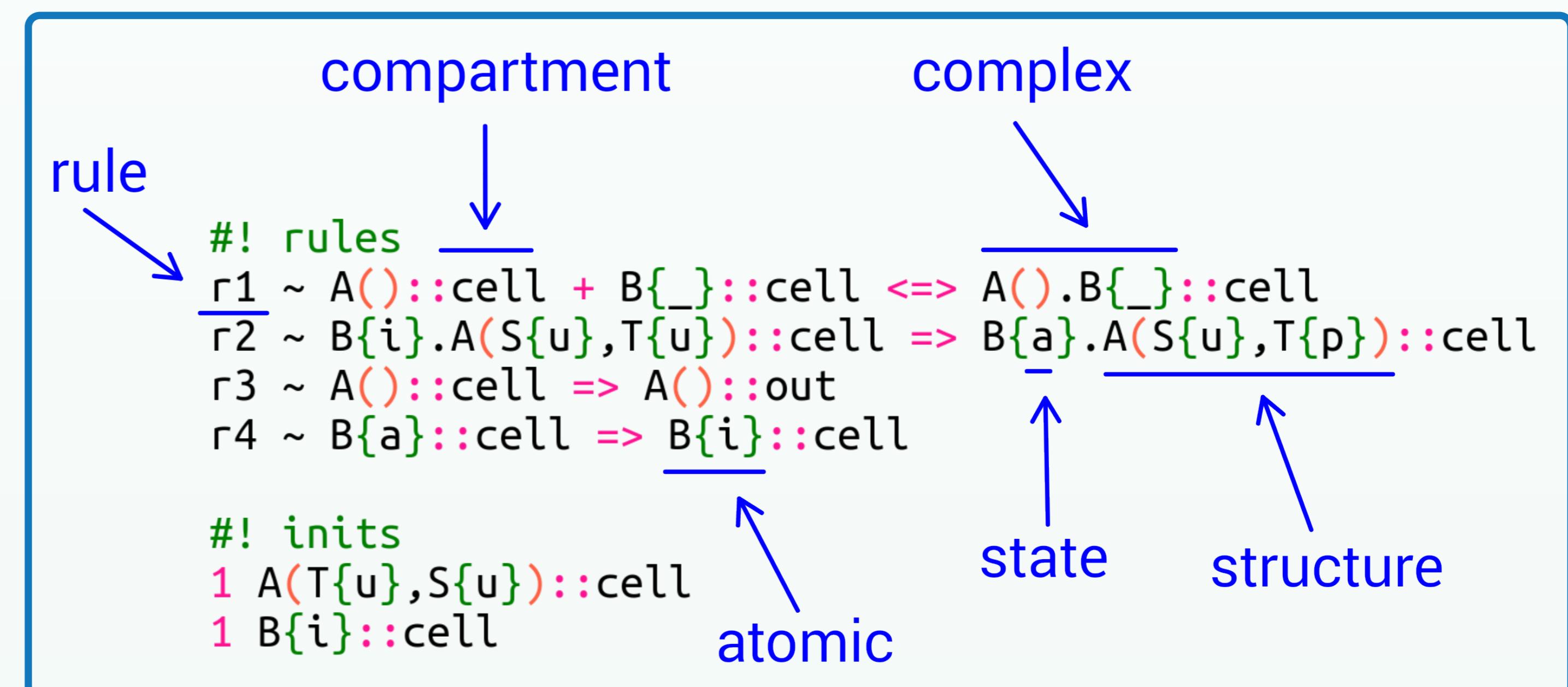
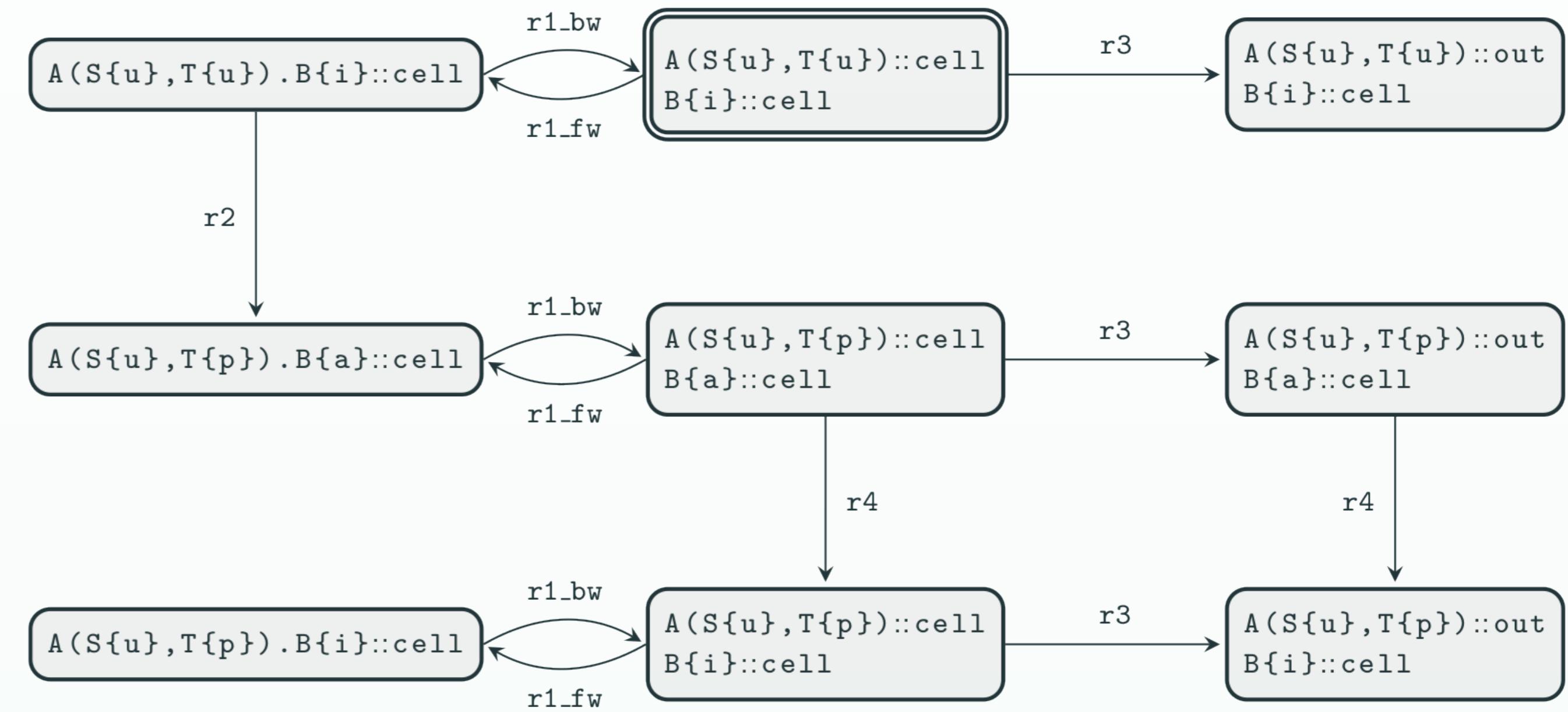
# Representing Biochemical Space Language in SBML-multi standard

Matej Troják, David Šafránek, Branislav Brozmann and Luboš Brim

Systems Biology Laboratory (SYBILA), Faculty of Informatics, Masaryk University, Brno, Czech Republic

Biochemical Space Language (BCSL) is a rule-based formalism developed for biological modelling and precise mechanistic annotation of existing mathematical models. With the focus on the usability by the users beyond computer science, it is also necessary to provide tools that enable efficient analysis techniques that help reveal inconsistencies in models and allow to analyse the modelled system's dynamics. To this end, it is crucial to support export to standard notation, enabling the importing of the model to external tools and broadening the available analysis toolset. In the case of rule-based languages, this is provided by the **SBML-multi** package. We implemented (partial) support for the export in our software tool **eBCSgen**. In this poster, we discuss the process of relating BCSL to SBML-multi, focusing on the raised issues and open problems.

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core"
      xmlns:multi="http://www.sbml.org/sbml/level3/version1/multi/version1"
      level="3" version="1" multi:required="true">
<model>
  <multi:listOfSpeciesTypes>
    <multi:speciesType multi:id="st_A_B_cell">
      <multi:listOfSpeciesTypeInstances>
        <multi:speciesTypeInstance multi:id="A_0" multi:speciesType="st_A"/>
        <multi:speciesTypeInstance multi:id="B_1" multi:speciesType="st_B"/>
      </multi:listOfSpeciesTypeInstances>
      <multi:listOfSpeciesTypeComponentIndexes>
        <multi:speciesTypeComponentIndex multi:id="A_0_S"
          multi:component="S" multi:identifyingParent="A_0"/>
        <multi:speciesTypeComponentIndex multi:id="A_0_T"
          multi:component="T" multi:identifyingParent="A_0"/>
      </multi:listOfSpeciesTypeComponentIndexes>
    </multi:speciesType>
  </multi:listOfSpeciesTypes>
  <listOfSpecies>
    <species id="sp_1223311970363763508" name="B{i}.A(S{u},T{u}):cell"
      compartment="cell" initialAmount="0" hasOnlySubstanceUnits="false"
      boundaryCondition="false" constant="false" multi:speciesType="st_A_B_cell">
      <multi:listOfSpeciesFeatures>
        <multi:speciesFeature multi:speciesFeatureType="S_feature_type"
          multi:occur="1" multi:component="A_0_S">
          <multi:listOfSpeciesFeatureValues>
            <multi:speciesFeatureValue multi:value="S_u"/>
          </multi:listOfSpeciesFeatureValues>
        </multi:speciesFeature>
        <multi:speciesFeature multi:speciesFeatureType="T_feature_type"
          multi:occur="1" multi:component="A_0_T">
          <multi:listOfSpeciesFeatureValues>
            <multi:speciesFeatureValue multi:value="T_u"/>
          </multi:listOfSpeciesFeatureValues>
        </multi:speciesFeature>
        <multi:speciesFeature multi:speciesFeatureType="B_feature_type"
          multi:occur="1">
          <multi:listOfSpeciesFeatureValues>
            <multi:speciesFeatureValue multi:value="B_i"/>
          </multi:listOfSpeciesFeatureValues>
        </multi:speciesFeature>
      </multi:listOfSpeciesFeatures>
    </species>
    ...
  </listOfSpecies>
  ...
  <listOfReactions>
    <reaction id="rc_4" name="r2 ~ B{i}.A(S{u},T{u}):cell => B{a}.A(S{u},T{p}):cell"
      reversible="false" fast="false">
      <listOfReactants>
        <speciesReference species="sp_1223311970363763508"
          stoichiometry="1" constant="false"/>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="sp_2210355731928925978"
          stoichiometry="1" constant="false"/>
      </listOfProducts>
    </reaction>
    ...
  </listOfReactions>
</model>
</sbml>
```



Abstraction employed in BCSL introduces non-trivial isomorphism which is not easy to capture on the level of SBML. We have identified three types of possible isomorphism occurring in a model:

- simple shuffling of identical agents

$A(\text{dom}[u]).B() \Rightarrow A(\text{dom}[p]).B()$   
 $B().A(\text{dom}[u]) \Rightarrow B().A(\text{dom}[p])$

- shuffling of compatible agents

$A(\text{dom}[u]).B() \Rightarrow A(\text{dom}[p]).B()$   
 $B().A() \Rightarrow B().A + A()$

- multiple domains in a structure agent within incompatible complexes

$A(S\{u\}, T\{p\}).B() \Rightarrow A(S\{p\}, T\{p\}).B()$   
 $A(T\{u\}, S\{u\}) \Rightarrow A(T\{p\}, S\{u\})$

