Representing Biochemical Space Language in SBML-multi standard

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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.

```
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      <multi:speciesType multi:id="st_A_B_cell">
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        </multi:listOfSpeciesTypeInstances>
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        </multi:listOfSpeciesTypeComponentIndexes>
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    </multi:listOfSpeciesTypes>
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       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"</pre>
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            <multi:listOfSpeciesFeatureValues>
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            </multi:listOfSpeciesFeatureValues>
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     </species>
    </list0fSpecies>
    t0fReactions>
     <reaction id="rc_4" name="r2 \tilde{B}_{i}.A(S_{u},T_{u})::cell => B_{a}.A(S_{u},T_{p})::cell
      reversible="false" fast="false">
        <speciesReference species="sp_1223311970363763508"</pre>
           stoichiometry="1" constant="false"/>
        </list0fReactants>
        t0fProducts>
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        </list0fProducts>
      </reaction>
    </listOfReactions>
  </model>
</sbml>
```

```
r3
                                                                     A(S{u},T{u})::out
                                      A(S\{u\},T\{u\})::cell
      A(S{u},T{u}).B{i}::cell
                                                                     B{i}::cell
                                       B{i}::cell
              r2
                               r1_bw
                                      A(S{u},T{p})::cell
                                                                     A(S{u},T{p})::out
      A(S{u},T{p}).B{a}::cell
                                                                     B{a}::cell
                                      B{a}::cell
                               r1_fw
                                                r4
                                                                          r4
                               r1_bw
                                                             r3
                                      A(S{u},T{p})::cell
                                                                     A(S{u},T{p})::out
      A(S{u},T{p}).B{i}::cell
                                                                     B{i}::cell
                                      B{i}::cell
                               r1_fw
                                                complex
               compartment
rule
        r1 ~ A()::cell + B{_}::cell <=> A().B{_}::cell r2 ~ B{i}.A(S{u},T{u})::cell => B{a}.A(S{u},T{p})::cell
         r3 ~ A()::cell => A()::out
         r4 ~ B{a}::cell => B{i}::cell
        #! inits
                                                    state
                                                                 structure
         1 A(T{u},S{u})::cell
         1 B{i}::cell
                                     atomic
```

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

 $A(dom\{u\}).B()::cell \Rightarrow A(dom\{p\}).B()::cell$ $B().A(dom\{u\})::cell \Rightarrow B().A(dom\{p\})::cell$

• shuffling of compatible agents

 $A(dom\{u\}).B()::cell \Rightarrow A(dom\{p\}).B()::cell$ $B().A()::cell \Rightarrow B()::cell + A()::cell$

• multiple domains in a structure agent within incompatible complexes

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



