

Multi-component multistate species in SBML

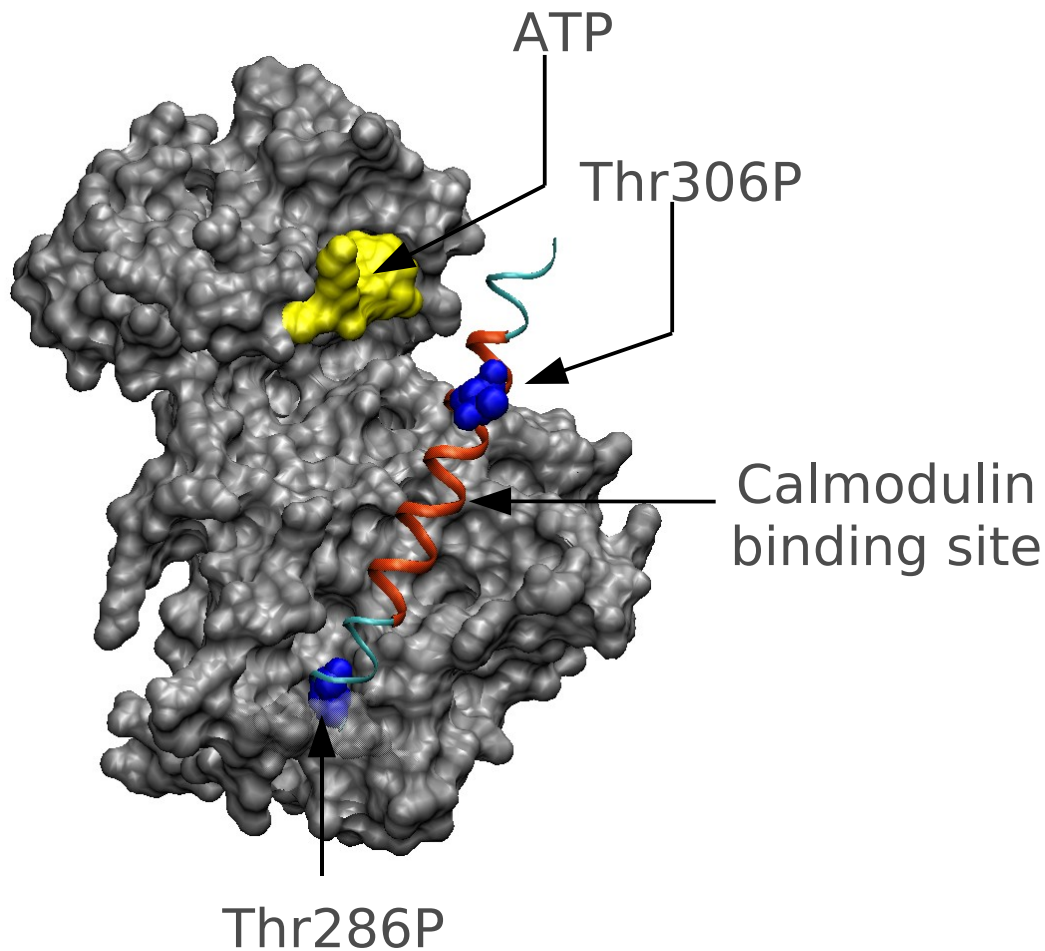
January 31st, 2008, Okinawa

Anika Oelrich, Software Engineer
EBI, WT Genome Campus
Hinxton, Cambridge, U.K.

EMBL-EBI

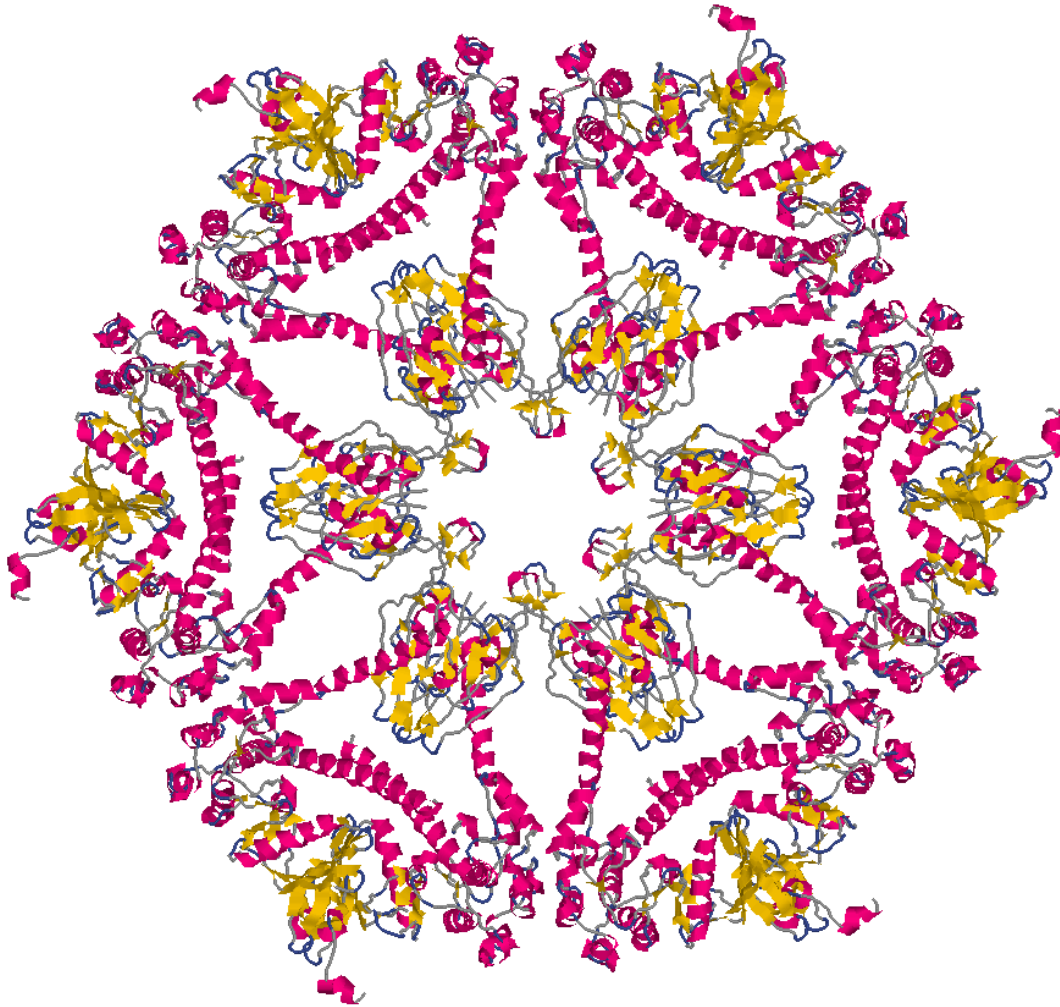


Multistate species



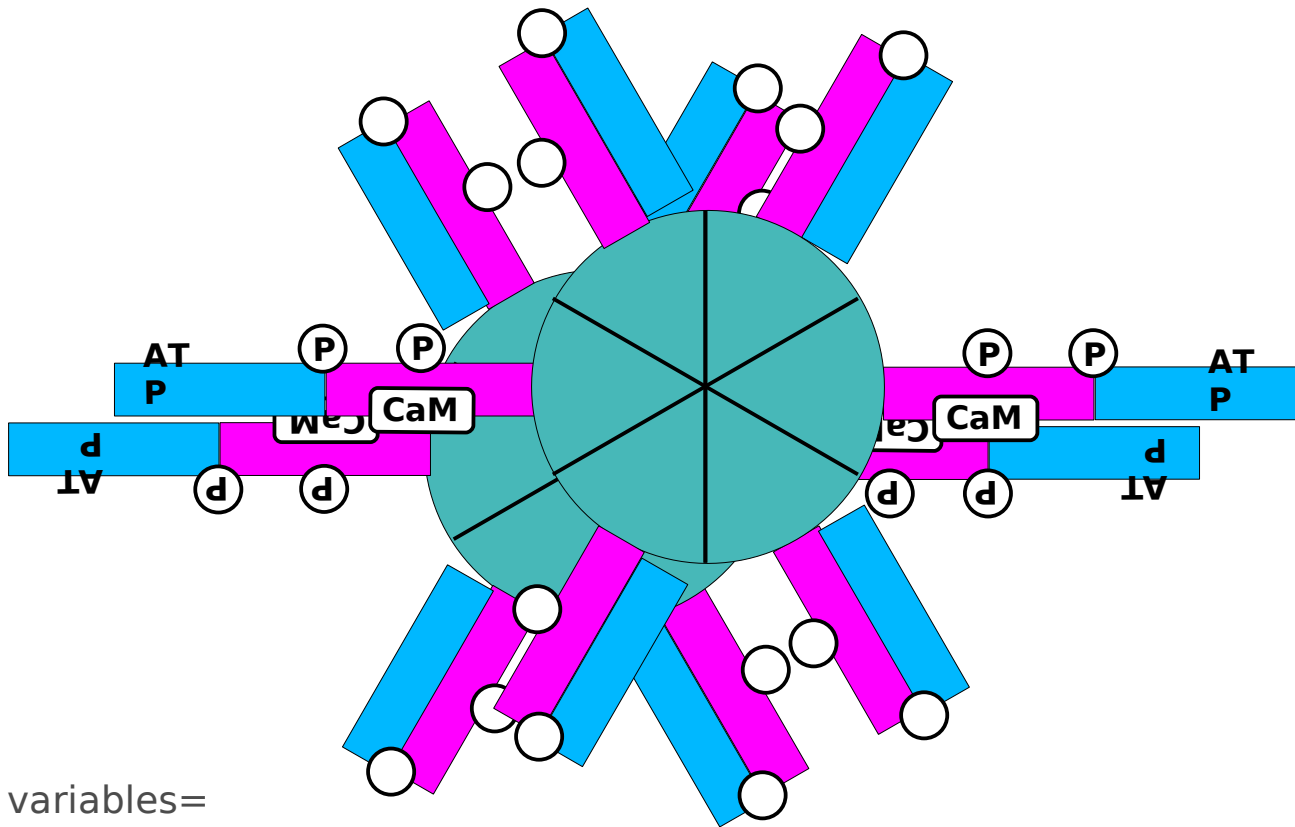
- state of a molecule depends on state variables
- state = (ATP, Thr306P, CaM, Thr286P, Activity)

Multi-component multistate species



- each component has state variables and binding sites
- whole hexamer has state variables and binding sites

Combinatorial explosion

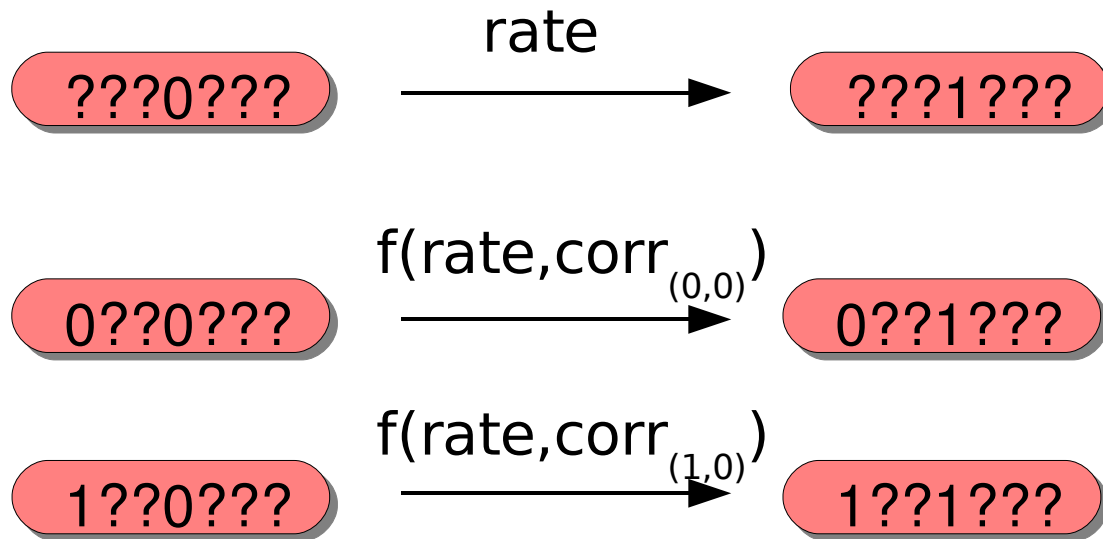


5x12 state variables=

1 152 900 000 000 000 000 states

(1 billion of billion)

Number of reactions

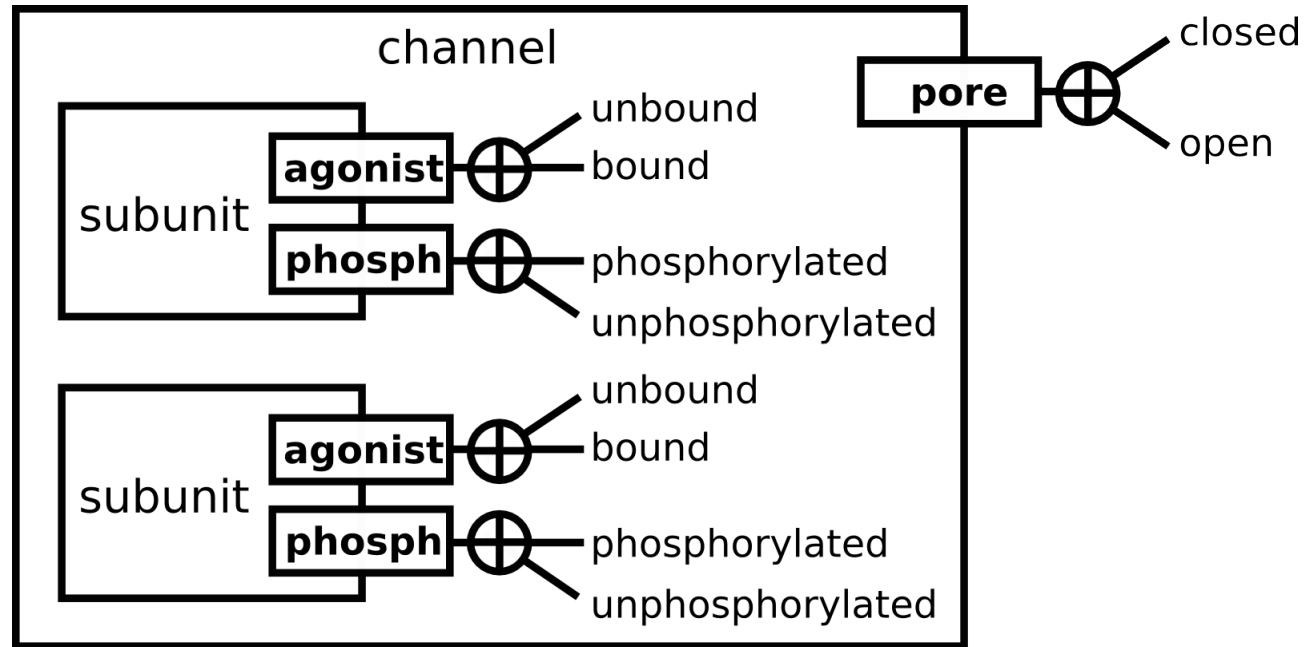


- only 4 states instead of 128
- only 2 reactions instead of 64

Multistate proposal

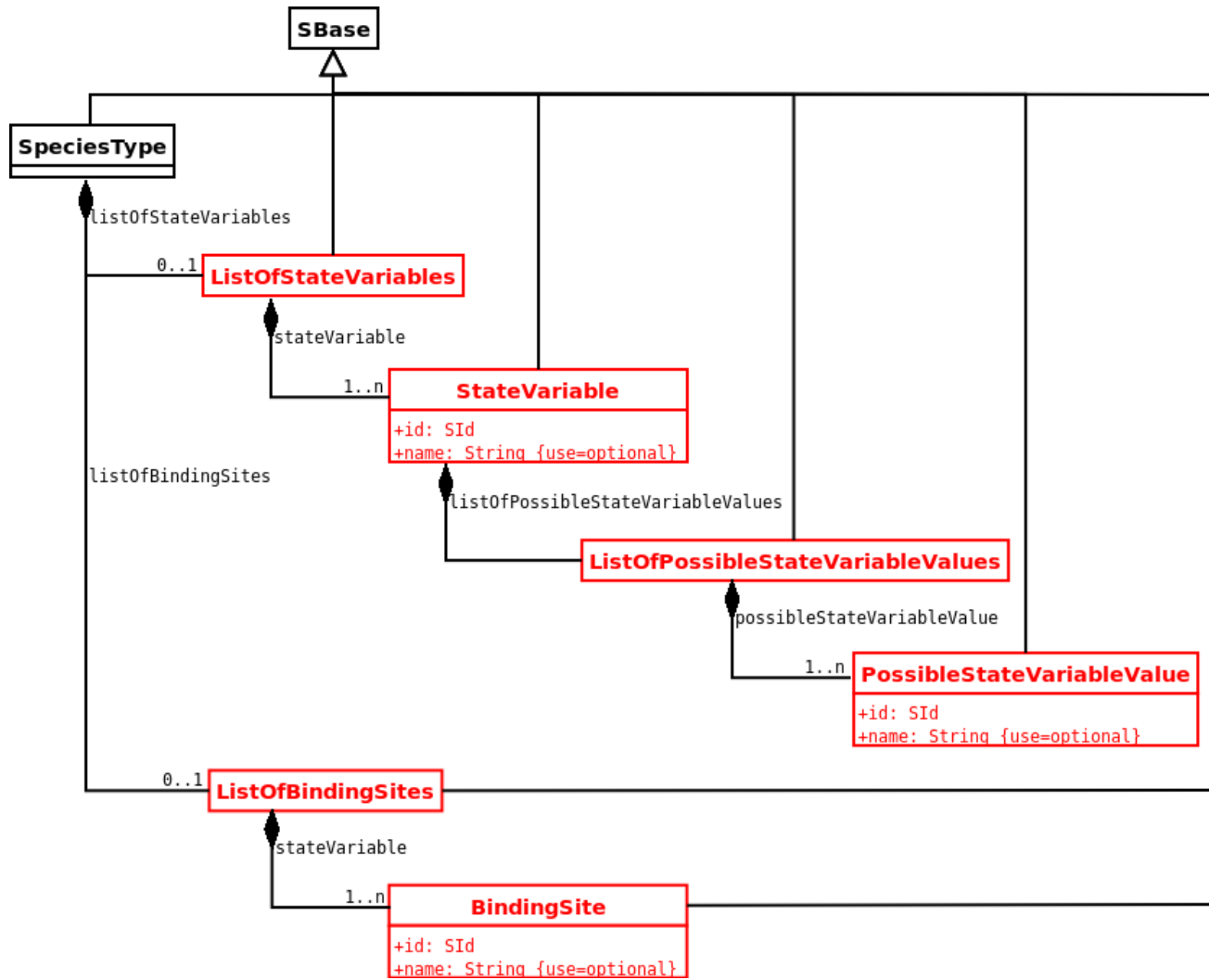
- ~10 months work
- Based on the proposals of Le Novère (2002), Finney (2004) and Blinov et al. (2006/2007)
- Following slides about the outcome of the last meeting 6th/7th December 2007 (Video conference workshop for L3M)

L3M extension - elements



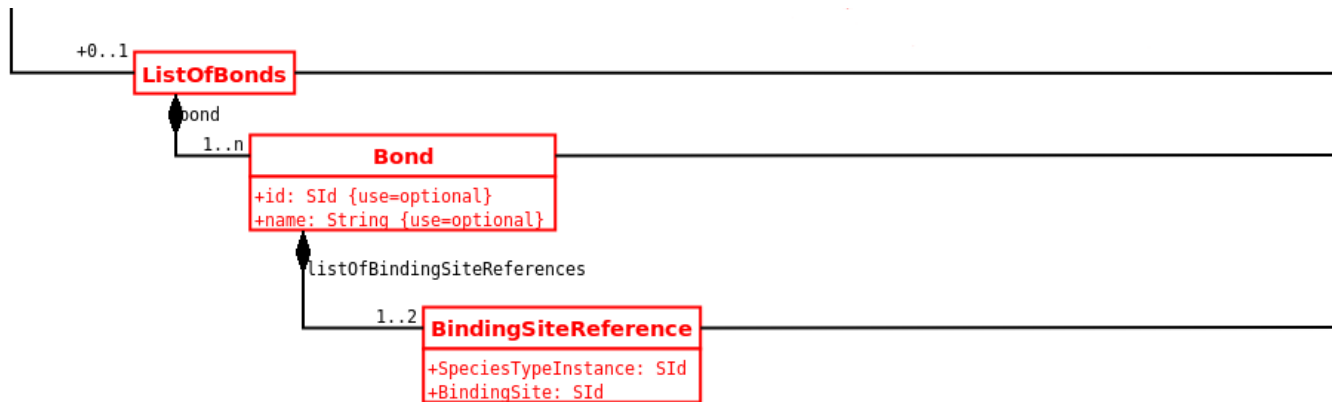
- extension: SpeciesType, Species, Reaction
- new element: Selector, ReactionRule

SpeciesType



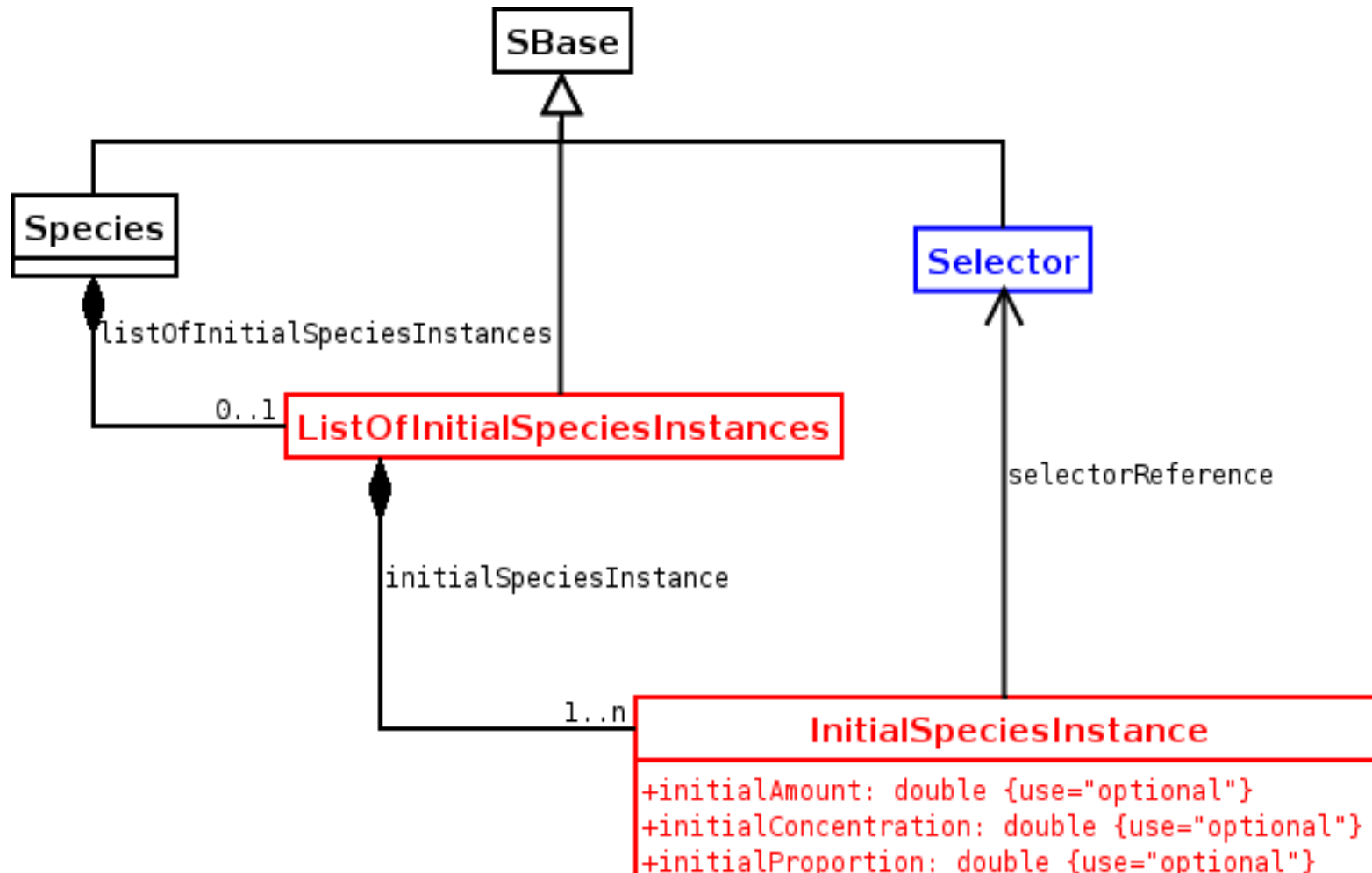
SpeciesType - example

```
<speciesType id="cyclin" >
  <l3m:listOfStateVariables>
    <l3m:stateVariable="phosphorylation" >
      <l3m:listOfPossibleStateVariableValues>
        <possibleStateVariableValue id="unphos" name="non-phosphorylated"/>
        <possibleStateVariableValue id="phos" name="phosphorylated" />
      </l3m:listOfPossibleStateVariableValues>
    </l3m:stateVariable>
  </l3m:listOfStateVariables>
  <l3m:listOfBindingSites>
    <l3m:bindingSite id="KSite" />
    <l3m:bindingSite id="CSite" />
  </l3m:listOfBindingSites>
</speciesType>
```

Selector - example

```
<l3m:selector id="scyclin">  
  <l3m:listOfSpeciesTypeInstances>  
    <l3m:speciesTypeInstance id="icyclin" speciesType="cyclin">  
      <l3m:listOfStateVariableInstances>  
        <l3m:stateVariableInstance stateVariable="phosphorylation" >  
          <l3m:listOfStateVariableValues>  
            <l3m:stateVariableValue possibleStateVariableValue="phos" />  
          </l3m:listOfStateVariableValues>  
        </l3m:stateVariableInstance>  
      </l3m:listOfStateVariableInstances>  
    </l3m:speciesTypeInstance>  
  </l3m:listOfSpeciesTypeInstances>  
  <l3m:listOfBonds>  
    <l3m:genericBond>  
      <l3m:bindingSiteReference speciesTypeInstance="icyclin" bindingSite="Ksite" />  
    </l3m:genericBond>  
  </l3m:listOfBonds>  
</l3m:selector>
```



Species - example

```
<species id="spcyclin" speciesType="cyclin" initialAmount="300">
  <l3m:listOfInitialSpeciesInstances>
    <l3m:initialSpeciesInstance id="" proportion="0.3">
      <l3m:selectorReference selector="scyclin_1" />
    </l3m:initialSpeciesInstance>
    <l3m:initialSpeciesInstance id="" proportion="0.7">
      <l3m:selectorReference selector="scyclin_2" />
    </l3m:initialSpeciesInstance>
  </l3m:listOfInitialSpeciesInstances>
</species>
```

- ReactionRules which will call Selectors and are connected to a specific reaction

How it looks like: ??? (we are currently working one ... 😊)

Thanks for your attention!