Managing Multiple Parameter Sets

Frank T. Bergmann (fbergman@u.washington.edu)

About this Document

This document describes the elements of a SBML annotation, for storing multiple parameter sets in an SBML model. A user might wish to store different parameter sets that exhibit interesting behavior of computational models. One common example would be to store parameter values for steady states, or even oscillating regimes.

The Annotation

The annotation itself could not be simpler and can be summarized in a brief snippet of XML like this:

```
<listOfParameterSets xmlns="http://sys-bio.org/ParameterSets" active="test">
        <parameterSet id="test" name="Test Set" >
                <listOfParameters>
                        <parameter sbmlId="Node0" value="1"/>
                </listOfParameters>
        </parameterSet>
</listOfParameterSets>
```

Let us have a look at each element in turn.

Parameter

The Parameter object is what this extension is all about. With two attributes, sbmlId and value, we hold the id, of the SBML element for which a value is saved, and the actual value. If needed, one could envision a subclass of Parameter that would hold additionally a reaction id, to store local parameters.

ListOfParameters

The ListOfParameters element holds a list of all Parameter objects. It is not strictly necessary but follows the SBML style.

ParameterSet

The ParameterSet element follows the usual SBML style of classes. It would inherit from SBase, in order to attach notes in the form of XHTML to a <notes> element, additional processing instructions and meta information can be added to a <annotation> element, and a metaid attribute can be set.

Additionally, a parameter set has an id and name attribute that identifies it uniquely. And of course a parameter set holds the ListOfParameter object.

ListOfParameterSets

All ParameterSet elements are held in a ListOfParameterSets element, which also represents the annotation element for the SBML model. Thus the namespace needs to be defined here.

The only needed attribute is called “active” and marks the currently active parameter set. If not set the first parameter set is considered to be active.

Implementation

An implementation exists in the SBML Support .NET library as is distributed with current versions of SBW[1]. This library provides utility functions on top of the libSBML C# bindings among other things. The ParameterSets implementation also reads an existing JDesigner annotation for multiple parameter sets.

The library is currently used by Ben(Zai)Ten, a new graphical modeling environment, see the screenshot in the figure below.

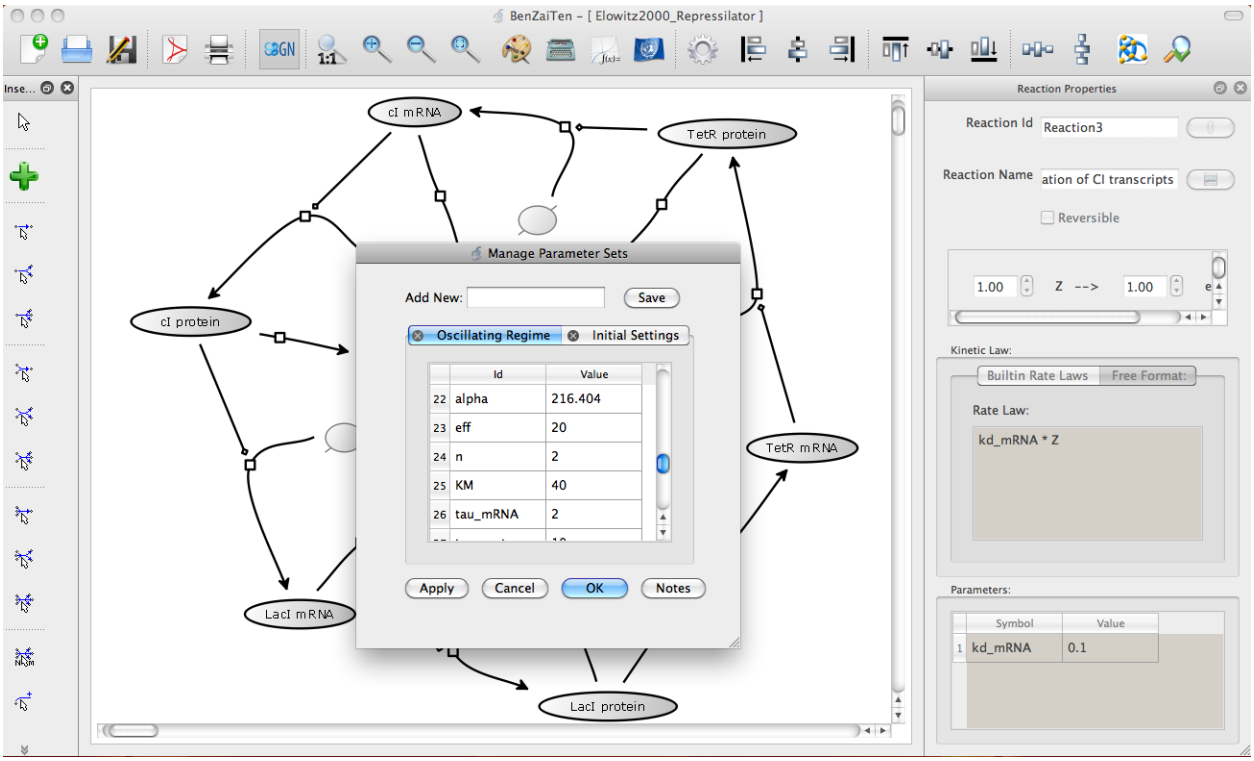

Figure 1: Multiple Parameter sets displayed for BioModel #12

Support for it is planned in the *Simulation Tool* and also the SED-ML prototypes will be able to construct changed models based in the different parameter sets.

[1] http://sys-bio.org/fbergman/files/latest/SetupSBW.exe

Example

Below an example of the Heinrich Oscillator with oscillating parameter regime and steady state:

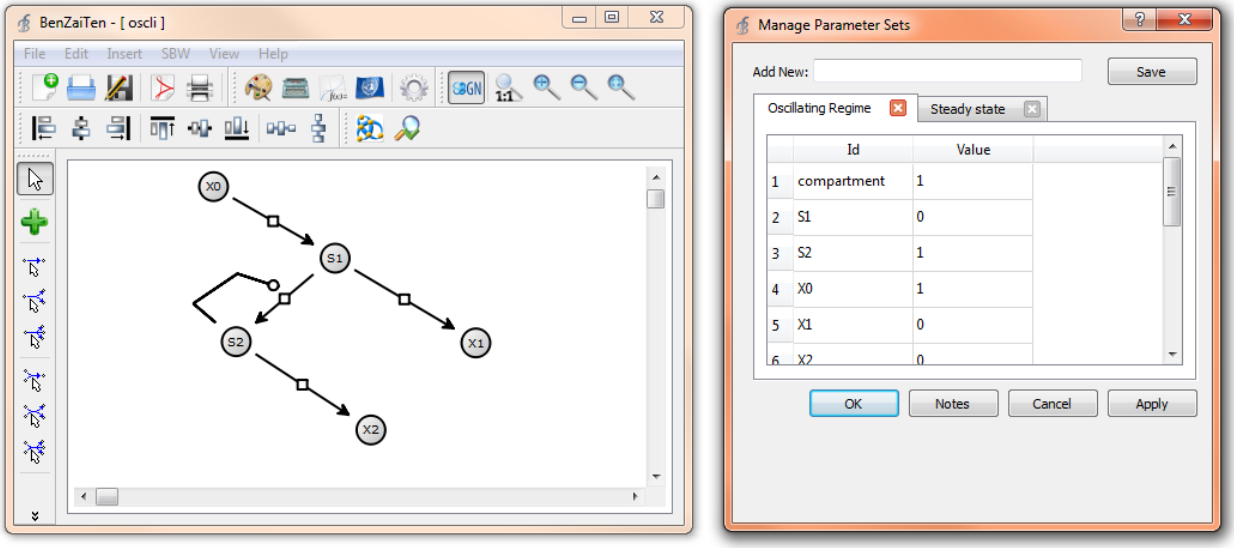

Figure 2: The Example in Ben(Zai)Ten

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns:jd2="http://www.sys-bio.org/sbml"
xmlns="http://www.sbml.org/sbml/level2/version4" level="2" version="4">
  <model id="oscli">
    <notes>
      <p xmlns="http://www.w3.org/1999/xhtml"/>
    </notes>
    <annotation>

      <listOfParameterSets xmlns="http://sys-bio.org/ParameterSets" active="oscil">
        <parameterSet id="oscil" name="Oscillating Regime">
          <parameter sbmlId="compartment" value="1"/>
          <parameter sbmlId="S1" value="0"/>
          <parameter sbmlId="S2" value="1"/>
          <parameter sbmlId="X0" value="1"/>
          <parameter sbmlId="X1" value="0"/>
          <parameter sbmlId="X2" value="0"/>
          <parameter sbmlId="J0_v0" value="8"/>
          <parameter sbmlId="J1_k3" value="0"/>
          <parameter sbmlId="J2_k1" value="1"/>
          <parameter sbmlId="J2_k_1" value="0"/>
          <parameter sbmlId="J2_c" value="1"/>
          <parameter sbmlId="J2_q" value="3"/>
          <parameter sbmlId="J3_k2" value="5"/>
        </parameterSet>
        <parameterSet id="steady" name="Steady state">
          <parameter sbmlId="compartment" value="1"/>
          <parameter sbmlId="S1" value="1.5699"/>
          <parameter sbmlId="S2" value="1.6"/>
          <parameter sbmlId="X0" value="1"/>
          <parameter sbmlId="X1" value="0"/>
          <parameter sbmlId="X2" value="0"/>
```

```
          <parameter sbmlId="J0_v0" value="8"/>
          <parameter sbmlId="J1_k3" value="0"/>
          <parameter sbmlId="J2_k1" value="1"/>
          <parameter sbmlId="J2_k_1" value="0"/>
          <parameter sbmlId="J2_c" value="1"/>
          <parameter sbmlId="J2_q" value="3"/>
          <parameter sbmlId="J3_k2" value="5"/>
        </parameterSet>
      </listOfParameterSets>
    </annotation>
    <listOfCompartments>
      <compartment id="compartment" size="1"/>
    </listOfCompartments>
    <listOfSpecies>
      <species id="S1" compartment="compartment" initialConcentration="0"/>
      <species id="S2" compartment="compartment" initialConcentration="1"/>
      <species id="X0" compartment="compartment" initialConcentration="1"
boundaryCondition="true"/>
      <species id="X1" compartment="compartment" initialConcentration="0"
boundaryCondition="true"/>
      <species id="X2" compartment="compartment" initialConcentration="0"
boundaryCondition="true"/>
    </listOfSpecies>
    <listOfParameters>
      <parameter id="J0_v0" value="8"/>
      <parameter id="J1_k3" value="0"/>
      <parameter id="J2_k1" value="1"/>
      <parameter id="J2_k_1" value="0"/>
      <parameter id="J2_c" value="1"/>
      <parameter id="J2_q" value="3"/>
      <parameter id="J3_k2" value="5"/>
    </listOfParameters>
    <listOfReactions>
      <reaction id="J0" reversible="false">
        <listOfReactants>
          <speciesReference species="X0"/>
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="S1"/>
        </listOfProducts>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <ci> J0_v0 </ci>
          </math>
        </kineticLaw>
      </reaction>
      <reaction id="J1" reversible="false">
        <listOfReactants>
          <speciesReference species="S1"/>
        </listOfReactants>
        <listOfProducts>
          <speciesReference species="X1"/>
        </listOfProducts>
        <kineticLaw>
          <math xmlns="http://www.w3.org/1998/Math/MathML">
            <apply>
              <times/>
              <ci> J1_k3 </ci>
```

```
        <ci> S1 </ci>
      </apply>
    </math>
  </kineticLaw>
</reaction>
<reaction id="J2" reversible="false">
  <listOfReactants>
    <speciesReference species="S1"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="S2"/>
  </listOfProducts>
  <kineticLaw>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply>
        <times/>
        <apply>
          <minus/>
          <apply>
            <times/>
            <ci> J2_k1 </ci>
            <ci> S1 </ci>
          </apply>
          <apply>
            <times/>
            <ci> J2_k_1 </ci>
            <ci> S2 </ci>
          </apply>
        </apply>
        <apply>
          <plus/>
          <cn type="integer"> 1 </cn>
          <apply>
            <times/>
            <ci> J2_c </ci>
            <apply>
              <power/>
              <ci> S2 </ci>
              <ci> J2_q </ci>
            </apply>
          </apply>
        </apply>
      </apply>
    </math>
  </kineticLaw>
</reaction>
<reaction id="J3" reversible="false">
  <listOfReactants>
    <speciesReference species="S2"/>
  </listOfReactants>
  <listOfProducts>
    <speciesReference species="X2"/>
  </listOfProducts>
  <kineticLaw>
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply>
        <times/>
        <ci> J3_k2 </ci>
```

```
              <ci> S2 </ci>
            </apply>
          </math>
        </kineticLaw>
      </reaction>
    </listOfReactions>
  </model>
</sbml>
```