1 Introduction

We present the Systems Biology Markup Language (SBML) Level 1, Version 2, a description language

tionally omitted from the language definition. Future software tools will undoubtedly require the evolution of SBML; we expect that subsequent releases of SBML (termed *levels*

reference is “http://www.mysim.org/ns” and the prefix is mysim. An example of an annotation might then be as follows:

```
...
<annotation  xmlns:mysim="http://www.mysim.org/ns">
      <mysim:nodecolors  mysim:bgcolor="green"  mysim:fgcolor="white"/>
      <mysim:timestamp>2000-12-18  18:31  PST</mysim:timestamp>
</annotation>
...
```

The namespace prefix mysim is used to qualify the XML elements mysim:nodecolors and mysim:timestamp;

```
letter   ::= 'a'..'z','A'..'Z'
digit    ::= '0'..'9'
name     ::= ( letter | '_' ) ( letter | digit | '_' )*
```

Figure 3: *The definition of the type SName, expressed in the variant of Extended Backus-Naur Form (EBNF) used by the*

The namespace rules described here provide a clean transition path to future levels of SBML, when submode6s

4 SBML Components

4.2 Unit Definitions

Units may be supplied in a number of contexts in an SBML model. A facility for defining units is convenient

possible to determine purely from the reaction equations whether one compartment is meant to be located within another. In the absence of a value for `outside`, compartment definitions in SBML Level 1 do not have any implied spatial relationships between each other.

In an XML data stream containing an SBML model, compartments are listed inside an XML element called `listOfCompartments` within a `Model`

The optional boolean field `boundaryCondition` determines whether the amount of the species is fixed or variable over the course of a simulation. The value of `boundaryCondition` defaults to "`false`", indicating that by default, the amount is not fixed. If the amount of a species is defined as being fixed, it implies that some external mechanism maintains a constant quantity in the compartment throughout the course of a reaction. (The term *boundary condition* alludes to the role of this constraint in a simulation.)

The optional field `charge` is an integer indicating the charge on the species (in terms of electrons, not the SI unit Coulombs). This may be useful when the species involved is a charged ion such as calcium (Ca^{2+}).

The fol1unda87-17.53ns221xampl(e)-42516(shda87-s53ns2228(y)w)(o)-2JET1001-2330562417.532cmBT0.890.940.28k00.890.9

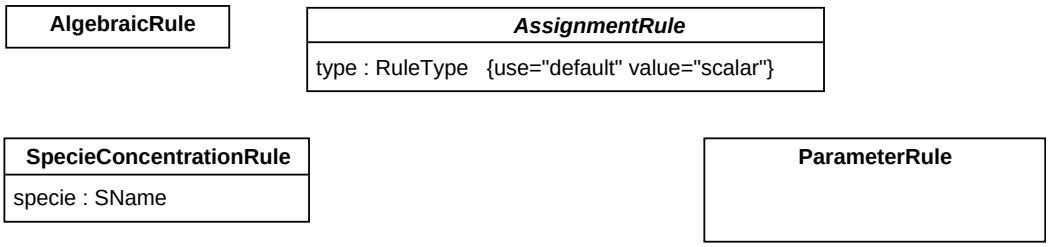

Figure 9: *The definition of* `Rule`

The effect of this rule depends on the value of the `type` field in `AssignmentRule`: if the type is "`scalar`", the rule sets the referenced parameter's value to that determined by the formula in `math`; if the type is "`rate`", the rule sets the rate of change of the parameter's value to that determined by the formula.

4.6.5 Constraints on rules

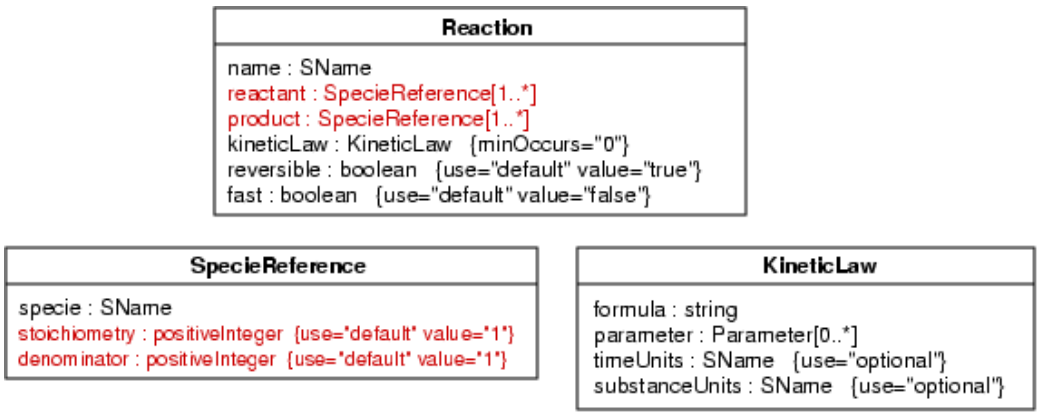

Figure 10: *The definitions of* `Reaction`, `KineticLaw` *and* `SpeciesReference`.

The field `fast` is another boolean attribute in the `Reaction` data structure; a value of "`true`" signifies that the given reaction is a "fast" one. This may be relevant when computing equilibrium concentrations of rapidly equilibrating reactions. Simulation/analysis packages may chose to use this information to reduce the number of ODEs required and thereby optimize such computations. The default value of `fast` is "`false`". (A simulator/analysis package that has no facilities for dealing with fast reactions can ignore this attribute. In theory, if the choice of which reactions are fast is correctly made, then a simulation performed with them

4.7.2 KineticLaw

A kineticLaw

```
                </listOfProducts>
                <kineticLaw formula="k4 * s2"/>
            </reaction>
        </listOfReactions>
    </model>
</sbml>
```

6 Discussion

```
  <xsd:restriction base="xsd:string">
    <xsd:pattern value="(_|[a-z]|[A-Z])(_|[a-z]|[A-Z]|[0-9])*"/>
  </xsd:restriction>
</xsd:simpleType>
<!--The definition of SBase follows.-->
<xsd:complexType name="SBase" abstract="true">
  <xsd:annotation>
    <xsd:documentation>The SBase type is the base type of all main
    components in SBML.  It supports attaching notes and annotations to
    components.</xsd:documentation>
  </xsd:annotation>
  <xsd:sequence>
    <xsd:element name="notes" minOccurs="0">
      <xsd:complexType>
```

```
</xsd:simpleType>
<!--The definition of Unit follows.-->
<xsd:complexType name="Unit">
  <xsd:complexContent>
    <xsd:extension base="SBase">
      <xsd:attribute name="kind" type="UnitKind" use="required"/>
      <xsd:attribute name="exponent" type="xsd:integer" default="1"/>
      <xsd:attribute name="scale" type="xsd:integer" default="0"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!--The definition of UnitDefinition follows.-->
<xsd:complexType name="UnitDefinition">
  <xsd:complexContent>
    <xsd:extension base="SBase">
      <xsd:sequence>
        <xsd:element name="listOfUnits" minOccurs="0">
          <xsd:complexType>
            <xsd:sequence>
              <xsd:element name="unit" type="Unit" maxOccurs="unbounded"/>
            </xsd:sequence>
          </xsd:complexType>
        </xsd:element>
      </xsd:sequence>
      <xsd:attribute name="name" type="SName" use="required"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!--The definition of Compartment follows.-->
<xsd:complexType name="Compartment">
  <xsd:complexContent>
    <xsd:extension base="SBase">
      <xsd:attribute name="name" type="SName" use="required"/>
      <xsd:attribute name="volume" type="xsd:double" default="1"/>
      <xsd:attribute name="units" type="SName" use="optional"/>
      <xsd:attribute name="outside" type="SName" use="optional"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!--The definition of Species follows.-->
<xsd:complexType name="Species">
  <xsd:complexContent>
    <xsd:extension base="SBase">
      <xsd:attribute name="name" type="SName" use="required"/>
      <xsd:attribute name="compartmen5(type="Unit)-SName" use="optional"/>
      <xsd:attribute name="initialAmoun5(type="Unit)-xsd:double" use="required"/>
      <xsd:attribute name="units" type="SName" use="optional"/>
      <xsd:attribute name="boundaryCondition(type="Unit)-xsd:boolean" use="optional" default="false"/>
      <xsd:attribute name="charge" type="xsd:integer" use="optional"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!--The definition of Parameter follows.-->
<xsd:complexType name="Parameter">
  <xsd:complexContent>
    <xsd:extension base="SBase">
      <xsd:attribute name="name" use="required"/>
      <xsd:attribute name="value" type="xsd:double" use="optional"/>
      <xsd:attribute name="units" type="SName" use="optional"/>
    </xsd:extension>
  </xsd:complexContent>
</xsd:complexType>
<!--The definition of Rule follows. -->
<xsd:simpleType name="RuleType">
  <xsd:restriction base="xsd:string">
    <xsd:enumeration value="scalar"/>
    <xsd:enumeration value="rate"/>
  </xsd:restriction>
</xsd:simpleType>
```

```
</xsd:sequence></xsd:complexType></xsd:element><xsd:element name="listOfParameters" minOccurs="0"><xs
```

C Predefined Functions in SBML

Table 6 lists the basic mathematical functions that are defined in SBML Level 1 at this time.

Name	Args.	Formula or Meaning	Argument Constraints	Result Constraints
abs	x	absolute value of x		
acos	x	arc cosine of x in radians	$-1.0 \leq x \leq 1.0$	$0 \leq acos(x) \leq \pi$
asin	x	arc sine of x in radians	$-1.0 \leq x \leq 1.0$	$-\pi/2 \leq asin(x) \leq \pi/2$
atan	x	arc tangent of x in radians		$-\pi/2 \leq atan(x) \leq \pi/2$
ceil	x			

Name	Arguments	Meaning	Formula
massi	S_i, k	Irreversible Mass Action Kinetics	$v = k \prod_i S_i$
massr	S_i, P_j, k_1, k_2	Reve.978rsible Mass Action Kinetics	$v = k_1 \prod_i S_i - k_2 \prod_j P_j$
uui	S, V_m, K_m	Irreversible Simple Michaelis-Menten	$v = \frac{V_m S}{}$

Name	Arguments	Meaning	Formula
uctr	S, P, A_c, V_f, V_r, K_{ms}, K_{mp}, K_a	Catalytic Activation (Reversible)	$v = \frac{V_f S/K_{ms} - V_r P/K_{mp}}{1 + K_a/A_c + (S/K_{ms} + P/K_{mp})(1 + K_a/A_c)}$
umai	S, A_c, V, K		

Symbol	Meaning
α	E□ect of S and P on binding of M (if $M < 1$, M is inhibitor; if $M > 1$, M is activator)
A	First substrate in two substrate reaction
A_c	Activator
B	Secbnd substrate in two substrate reaction
I	Inhibitor
K	

K

References