

XXML

und seine Untersprachen
CellML, CSML, SBML

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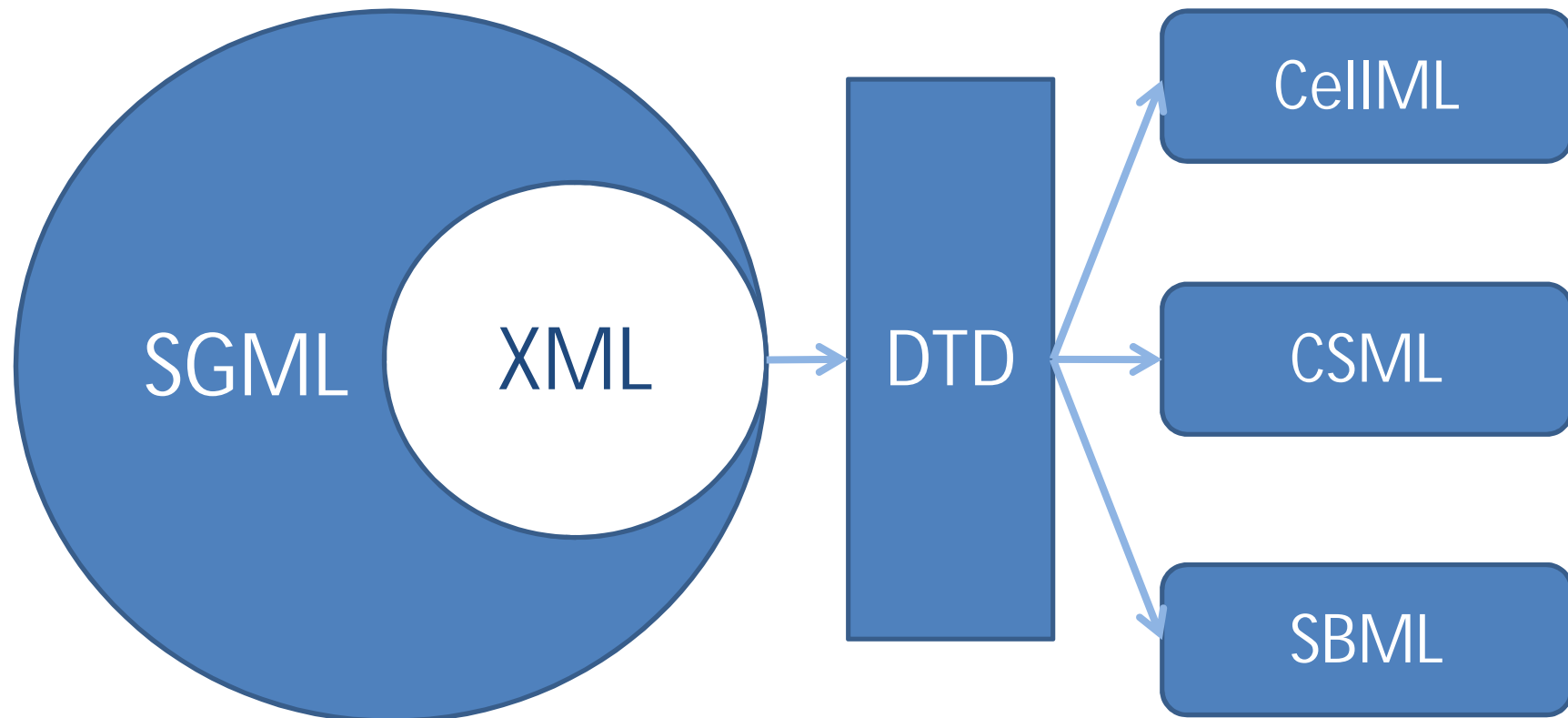
XML

CellML

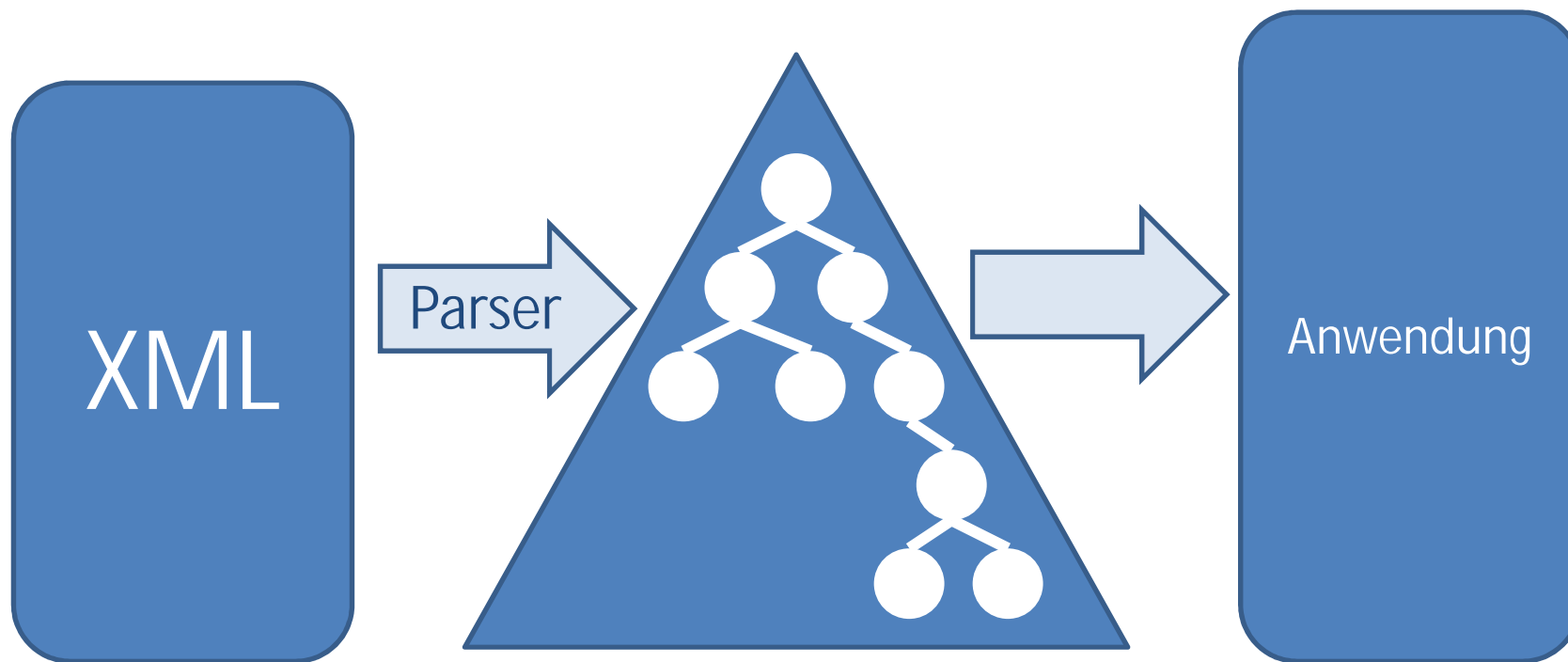
CSML

SBML

- n eXtensible Markup Language
- n XML ist eine Auszeichnungssprache
- n XML ist erweiterbar



- n XML stellt Vorschriften zur eigenen Typdefinition bereit
- n ein XML Dokument hat eine Baumstruktur



Aufbereitung der XML-Daten über eine Baumstruktur

n XML Syntax

Beschreibung	XML
Prolog und DTD-Definition	<code><?xml version="1.0"?></code> <code><!DOCTYPE ... ></code>
Elemente	<code><ELEMENT attribut ="Wert"> Inhalt</code> <code></ELEMENT></code>

n Elemente Dokumentstruktur

n Attribute spezifizieren Elemente

```
<AUTOR>
```

```
  <VORNAME> Hans </VORNAME>
```

```
  <NACHNAME> Heinrich </NACHNAME>
```

```
  < IMG quelle="bild.jpg" hoehe="200" breite="100"/>
```

```
</AUTOR>
```

- n DTD Document Type Definition
- n Sprache zur Definition von
Elementtypen, Attributen und Entities
innerhalb eines XML-Dokumentes

- n externe DTD

```
<!DOCTYPE model SYSTEM "http://www.cellml.org/cellml/cellml_1_1.dtd">  
<!DOCTYPE name SYSTEM "extern.dtd">
```

- n interne Definition

```
<!DOCTYPE MUSIKSAMMLUNG [  
  <!ELEMENT MUSIKSAMMLUNG (ALBUM+)  
  ...
```

n DTD

```
<!ELEMENT MUSIKSAMMLUNG (ALBUM+)>
```

```
<!ELEMENT ALBUM (AUTOR,  
                INTERPRET | SAENGER | SAENGERIN | GRUPPE),  
                TITEL,  
                LIED*)>
```

```
<!ELEMENT AUTOR (#PCDATA)>
```

```
<!ELEMENT LIED (#PCDATA)>
```

```
<!ATTLIST LIED
```

```
    tracknummer CDATA #REQUIRED
```

```
    kennung ID #IMPLIED >
```

```
    medium (DVD|CD|MD|HD) #REQUIRED >
```

XML

CellML

CSML

SBML



- n Cell Markup Language
- n beschreibt mathematische Modelle
- n wurde für das Physiome Project entwickelt
- n CellML bindet andere Sprachen ein:
 - MathML
 - RDS Resource Description Framework



n Metadata

CellML verwendet verschiedene Standards zur Metadaten Beschreibung:

RDF, Dublin Core, vCard, and BQS

```
<rdf:Description rdf:about=" „ ... ">  
  <dc:creator rdf:parseType="Resource">  
    <vCard:N rdf:parseType="Resource">  
      <vCard:Family>Lloyd</vCard:Family>  
      <vCard:Given>Catherine</vCard:Given>  
      <vCard:Other>May</vCard:Other>  
    </vCard:N>  
  </dc:creator>  
</rdf:Description>
```




n Units

Einheiten werden definiert basierend auf
SI International System of Units

```
<units name="millimolar">  
  <unit prefix="milli" units="mole" />  
  <unit units="litre" exponent="-1" />  
</units>
```



n Components, Variables and Equations

Komponente environment beinhaltet globale Variablen

```
<component name="environment">  
  <variable name="time" public_interface="out" units="second" />  
</component>
```

Gleichungen werden mit MathML beschrieben

```
<math>  
  <mi>x</mi>  
  <mo>=</mo>  
  <mfrac>
```



XML

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n Interfaces, Groups and Connections

Interface beschreibt Richtung des Variablen austausch

```
<component name="m_gate">  
  <variable name="m" public_interface="out" units="dimensionless" />  
</component>
```

```
<group choice="opt" rep="norepeat">  
  <relationship_ref relationship="encapsulation" />  
  <component_ref component="sodium_channel">  
    <component_ref component="m_gate" />  
    <component_ref component="h_gate" />  
  </component_ref></group>
```



n Interfaces, Groups and Connections

Connections mappen Variablen zweier Komponenten aufeinander

```
<connection>  
  <map_components component_1="sodium_channel"  
    component_2="m_gate" />  
  <map_variables variable_1="m" variable_2="m" />  
</connection>
```

XML

CellML

CSML

SBML



- n Cell System Markup Language
- n Format zur Visualisierung, Modellierung und Simulation von Biopathways
- n Erweitert CellML und SBML um Visualisierung



n CSML

Projekt: <project>

Model: <model>

Entity: <entity>

Process: <process>

Connector: <connector>

Fact: <fact>

Participant: <participant>

Set of Entity: <entitySet>

Set of Process: <processSet>

Set of Fact: <factSet>

Import: <importModel>

Map: <entityMap> <processMap>

Merge: <elementMerge>



n CSML Visualisierung

n View Property

View Property: <viewProperty>

Position: <position>

Shape: <shape>

SVG: <svg:svg>

Cache: <cache>

Global View Property: <globalViewProperty>

Global Shape: <globalShape>

n View Model Property

ViewSet: <viewSet>

View: <view>

Layout: <layout>

Reference Element: <refElement>



n CSML Visualisierung

n Chart Property

Chart Set: <chartSet>

Chart: <chart>

Property: <property>

Reference Chart Element: <refChartElement>

Reference Chart: <refChart>

n Animation Property

Global Animation Property: <globalAnimationProperty>

Global Animation: <globalAnimation>

Animation Property: <animationProperty>

Animation: <animation>



- n Systems Biology Markup Language
- n beschreibt Biochemische Reaktionsnetzwerke
- n Nutzt RDF und vCard zur Metadatenbeschreibung
- n Nutzt MathML für Gleichungen

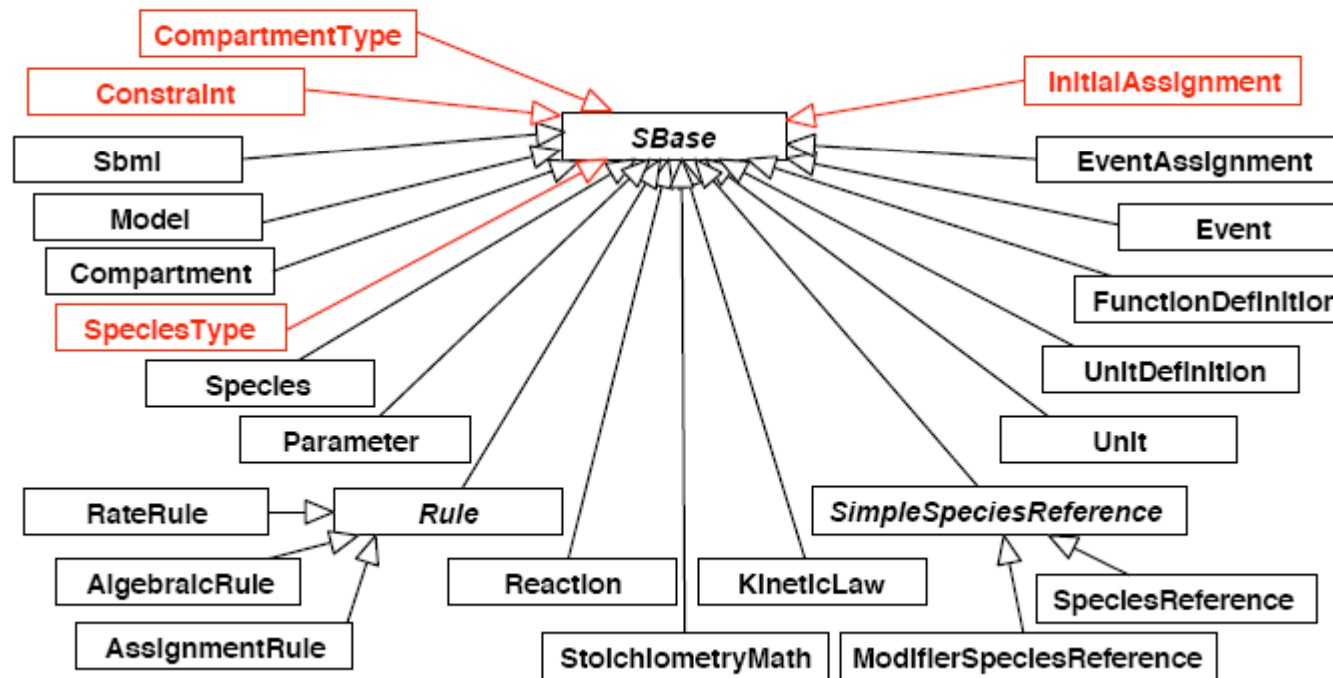


n Struktur

- beginning of model definition
- list of function definitions (optional)
- list of unit definitions (optional)
- list of compartment types (optional)
- list of species types (optional)
- list of compartments (optional)
- list of species (optional)
- list of parameters (optional)
- list of initial assignments (optional)
- list of rules (optional)
- list of constraints (optional)
- list of reactions (optional)
- list of events (optional)
- end of model definition



n Struktur





n Struktur

```
<reaction metaid="metaid_0000106" id="G1R_Binding" name="Binding of  
Rum1 to Cig2_Cdc2" reversible="false" fast="false">  
  <annotation> ... metadaten ... </annotation>  
  <listOfReactants>  
    <speciesReference species="G1K"/>  
    <speciesReference species="R"/>  
  </listOfReactants>  
  <listOfProducts>  
    <speciesReference species="G1R"/>  
  </listOfProducts>  
  <kineticLaw timeUnits="time" substanceUnits="substance">  
    <math ... > ... mathe ... </math>  
  </kineticLaw>  
</reaction>
```

Quellen

- n XML – Grundlagen – RRZN
- n CSML 3.0 – Basic Concepts and Specialisation
- n SBML - Structures and Facilities for Model Definitions
- n www.cellml.org
- n www.sbml.org
- n www.csml.org