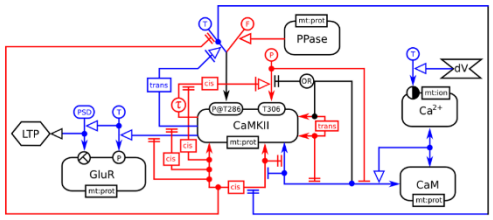
The Systems Biology Markup Language

SBML www.sbml.org

Why standards ?

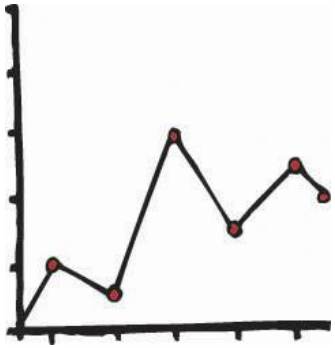
Software independent format



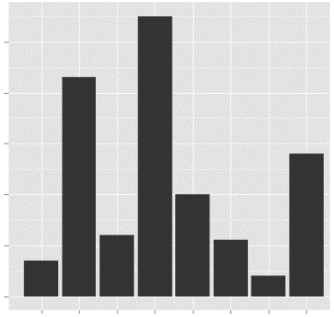
My model

His software

Her software



My results



Additional results

Why standards ?

Goal: reproducible and reusable models and simulations

- Need to capture both
  - **Mathematical** content
  - **Semantic** content
- Need a **software-independent** format

SBML is:

- A computer writable/readable file format for storing/exchanging biochemical models
- Expressed in XML
- It is developed by the community
- Free to use
- Widely supported (see list of supporting software on www.sbml.org)

The model

The basics, classical biochemical model:

- The **compartments** have a **volume** and contain metabolites
- The **species** have a **concentration**
- **Reactions** consume and produce substances and have a **reaction rate** (arbitrary kinetic functions)

Skeleton of an SBML file

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml
xmlns="http://www.sbml.org/sbml/level2/version3"
level="2" version="3">
<model id="Model_1" name="New Model">
<listOfCompartments>
...
</listOfCompartments>
<listOfSpecies>
...
</listOfSpecies>
<listOfReactions>
...
</listOfReactions>
</model>
</sbml>
```

The encoding

A **compartment** with an identifier and a size (volume):

```
<listOfCompartments>
  <compartment id="cell" name="cell" spatialDimensions="3" size="1" constant="true"/>
</listOfCompartments>
```

Species

A species is in a compartment

The amount of a species can be expressed in concentrations or amount of substance (hasOnlySubstanceUnits attribute)

The species´ concentration may be controlled by reactions or something else (boundaryCondition attribute)

```
<listOfSpecies>
  <species id="CSP" name="CSP" compartment="cell" initialConcentration="0.000652716"
boundaryCondition="false" constant="false"/>
  <species id="Pre_CSP" name="Pre_CSP" compartment="cell" initialConcentration="0.999999"
boundaryCondition="false" constant="false"/>
</listOfSpecies>
```

The details: reactions

- A reaction has substrates and product, possibly modifiers
- The kinetic law is written in MathML
- Kinetic parameter can be specified
- The units of the kinetic law is amount of substance per time (not concentration per time)

The important part about the reaction is the mathematical expression that describes how fast the reaction happens.

Reactions

```
<reaction id="reaction_1" name="reaction"
reversible="false">
<listOfReactants>
<speciesReference species="species_1"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="species_2"/>
</listOfProducts>
<kineticLaw>
<math
xmlns="http://www.w3.org/1998/Math/MathML">
<apply>
<times/>
<ci> compartment_1 </ci>
<ci> k1 </ci>
<ci> species_1 </ci>
</apply>
</math>
<listOfParameters>
<parameter id="k1" value="0.1"/>
</listOfParameters>
</kineticLaw>
</reaction>
```

Additional model elements

There are models that cannot be completely expressed using the compartment/species/reaction scheme.

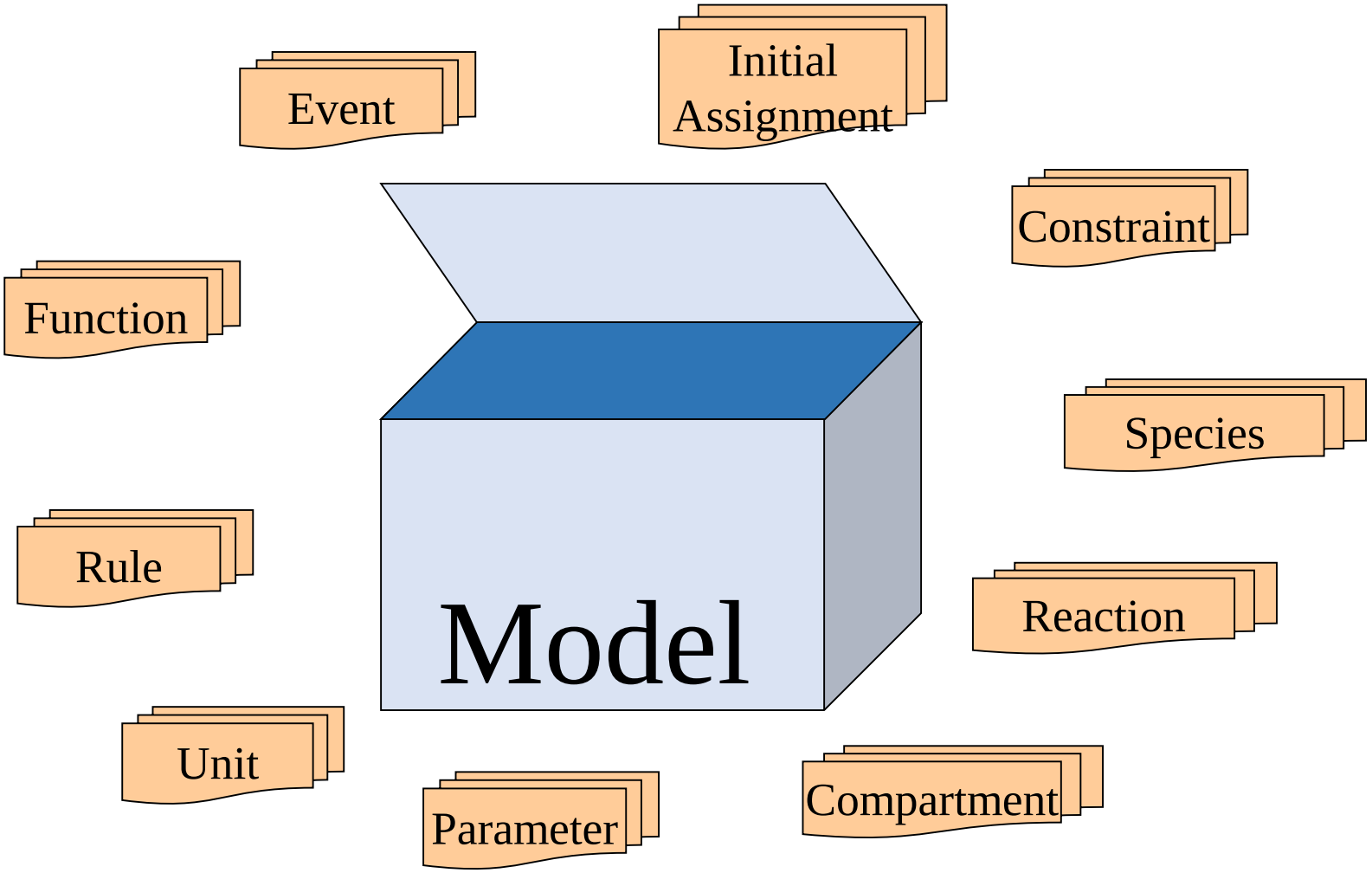
For this there are numerous constructs in SBML:

- Rules These can be used to define the value of objects (like species concentrations or compartment volumes). Rules can be algebraic assignments or differential equations (or implicit algebraic dependencies)

- Events These can change variables when a certain condition is fulfilled

- ….

SBML model elements



SBML organization

- SBML is a community effort.
- It is part of the COMBINE effort (co.mbine.org) with 2 international meetings every year
- SBML Team, SBML Editors, SBML Forum.