07: Systems Biology Markup Language (SBML)

https://github.com/matthiaskoenig/itbtechtalks

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Standard Formats

- Encoding of information in computer readable format
  - Minimal Information for models and simulation (MIRIAM, MIASE)

- Exchangeability & Reusability

- Reproducibility
  - Identical results with multiple simulators (roadrunner, COPASI, JWS)

- Annotations (to ontologies)
  - Knowledge integration (biological, computational)
  - Documentation (what is my model component)

- Quality
  - Automatic validation, e.g., model quality (unit checking, model consistency)

- Software & Tools
  - Simulation, Visualization, Analysis, Model Repositories, Parameter fitting
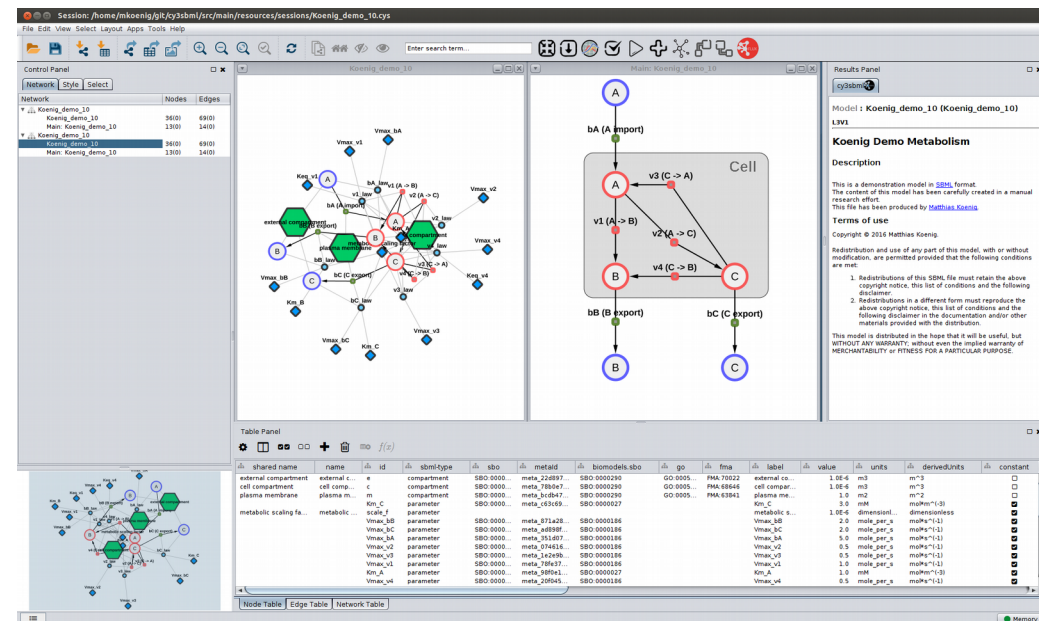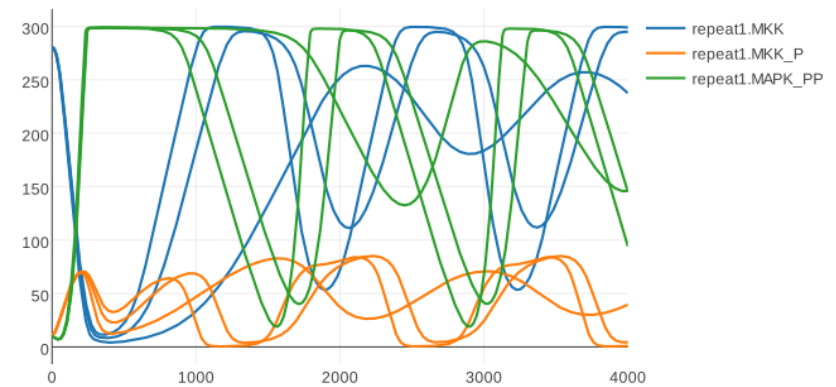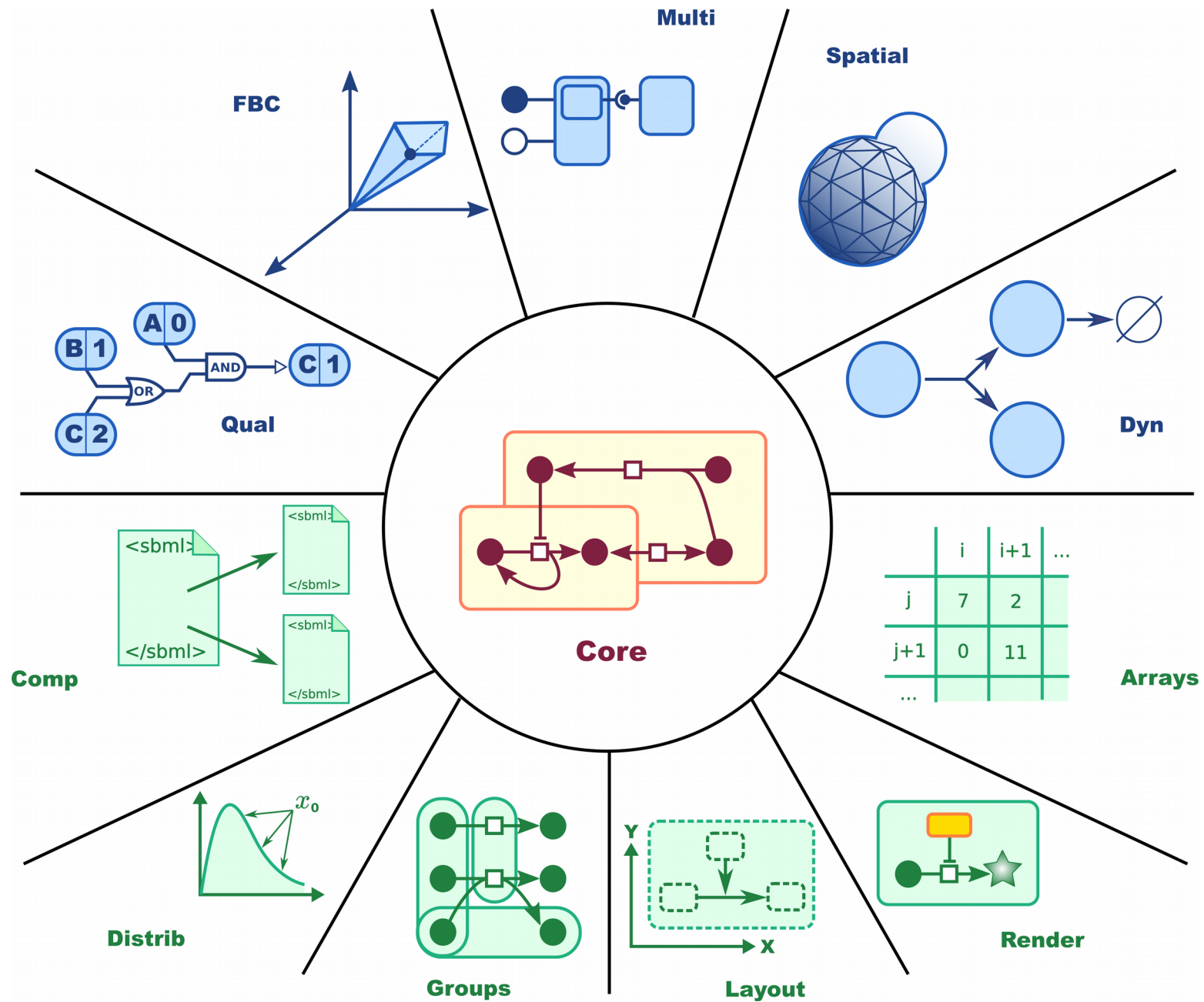
Systems Biology Markup Language

- De facto standard for encoding computational models (ODE)

- >280 software tools (simulation, visualization, parameter fitting, …)

- Model data bases Biomodels, JWS

- **libsbml**: LibSBML is a free, open-source programming library to read, write, manipulate, translate, and validate SBML files (C++, python, R, JavaScript, Matlab, Java, …)
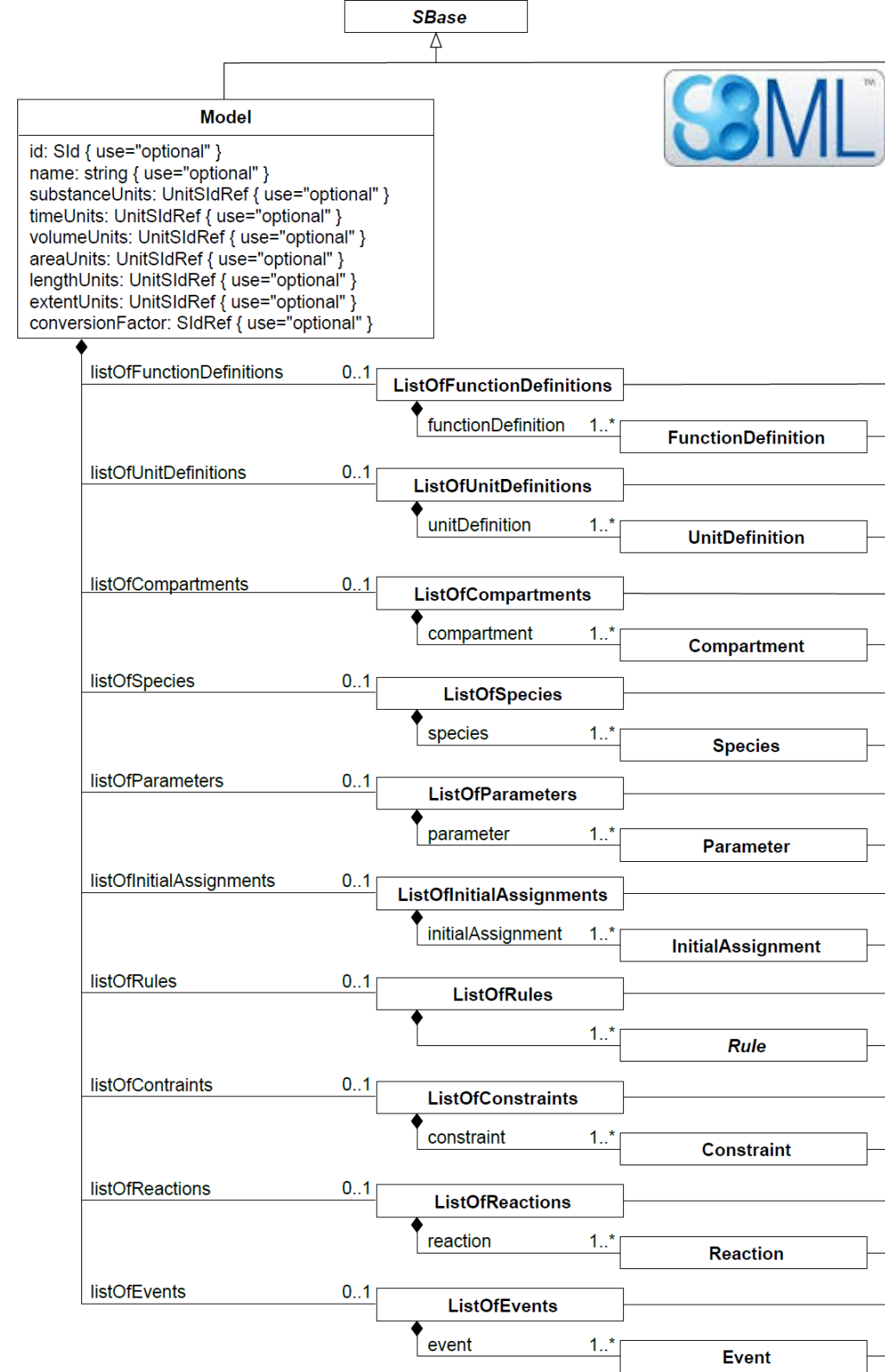
SBML Packages

A

```xml
<?xml version="1.0" encoding="UTF-8"?>
<sbml xmlns="http://www.sbml.org/sbml/level3/version1/core" level="3" version="1"
    xmlns:layout="http://www.sbml.org/sbml/level3/version1/layout/version1"
    layout:required="false">

    <model name="Tiny model example" >
    <listOfCompartments> ... </listOfCompartments>
    <listOfSpecies> ... </listOfSpecies>
    <listOfParameters> ... </listOfParameters>
    <listOfInitialAssignments> ... </listOfInitialAssignments>
    <listOfRules> ... </listOfRules>
    <listOfConstraints> ... </listOfConstraints>
    <listOfReactions> ... </listOfReactions>
    <listOfEvents> ... </listOfEvents>

    <layout:listOfLayouts xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" >
        <layout:layout layout:id="layout_1" layout:name="Layout">
            <layout:dimensions layout:width="620" layout:height="400"/>
            <layout:listOfCompartmentGlyphs> ... </layout:listOfCompartmentGlyphs>
            <layout:listOfSpeciesGlyphs> ... </layout:listOfSpeciesGlyphs>
            <layout:listOfReactionGlyphs> ... </layout:listOfReactionGlyphs>
            <layout:listOfTextGlyphs> ... </layout:listOfTextGlyphs>
        </layout:layout>
    </layout:listOfLayouts>
</model>
</sbml>
```

Labels (A): declaration of packages; variables; relationships; Core; Package; References

B

```xml
<compartment id="c" name="cell" size="1" constant="1">
<species metaid="S1" id="Glu" name="glucose"
        compartment="c" initialAmount="100" sboTerm="SBO:0000247"
        hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false"/>
<species metaid="S2" id="G6P" name="glucose 6 phosphate"
        compartment="c" initialAmount="0" sboTerm="SBO:0000247"
        hasOnlySubstanceUnits="false" boundaryCondition="false" constant="false" >
  <annotation>
    ...
    <bqbiol:isVersionOf>
    ...
            <rdf:li rdf:resource="http://identifiers.org/chebi/CHEBI:58247"/>
    ...
<parameter id="Vm" value="10" constant="true" sboTerm="SBO:0000186"/>
<parameter id="Km" value="10" constant="true" sboTerm="SBO:0000371"/>
<reaction id="R1" name="glucokinase" reversible="false">
    ...
    <speciesReference species="Glu" stoichiometry="1" constant="true" sboTerm="SBO:0000015"/>
    ...
    <speciesReference species="G6P" stoichiometry="1" constant="true" boTerm="SBO:0000011"/>
    ...
  <kineticLaw sboTerm="SBO:0000031">
    <math xmlns="http://www.w3.org/1998/Math/MathML">
      <apply>
        <divide />
        <apply>
          <times/>
          <ci> Vm </ci>
          <ci> Glu </ci>
        </apply>
    ...
```