

Numerical Markup Language (NuML) & Data Converter

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History of NuML

- Originated from numerical aspects of SBRML

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Systems biology

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SBRML: a markup language for associating systems biology data with models

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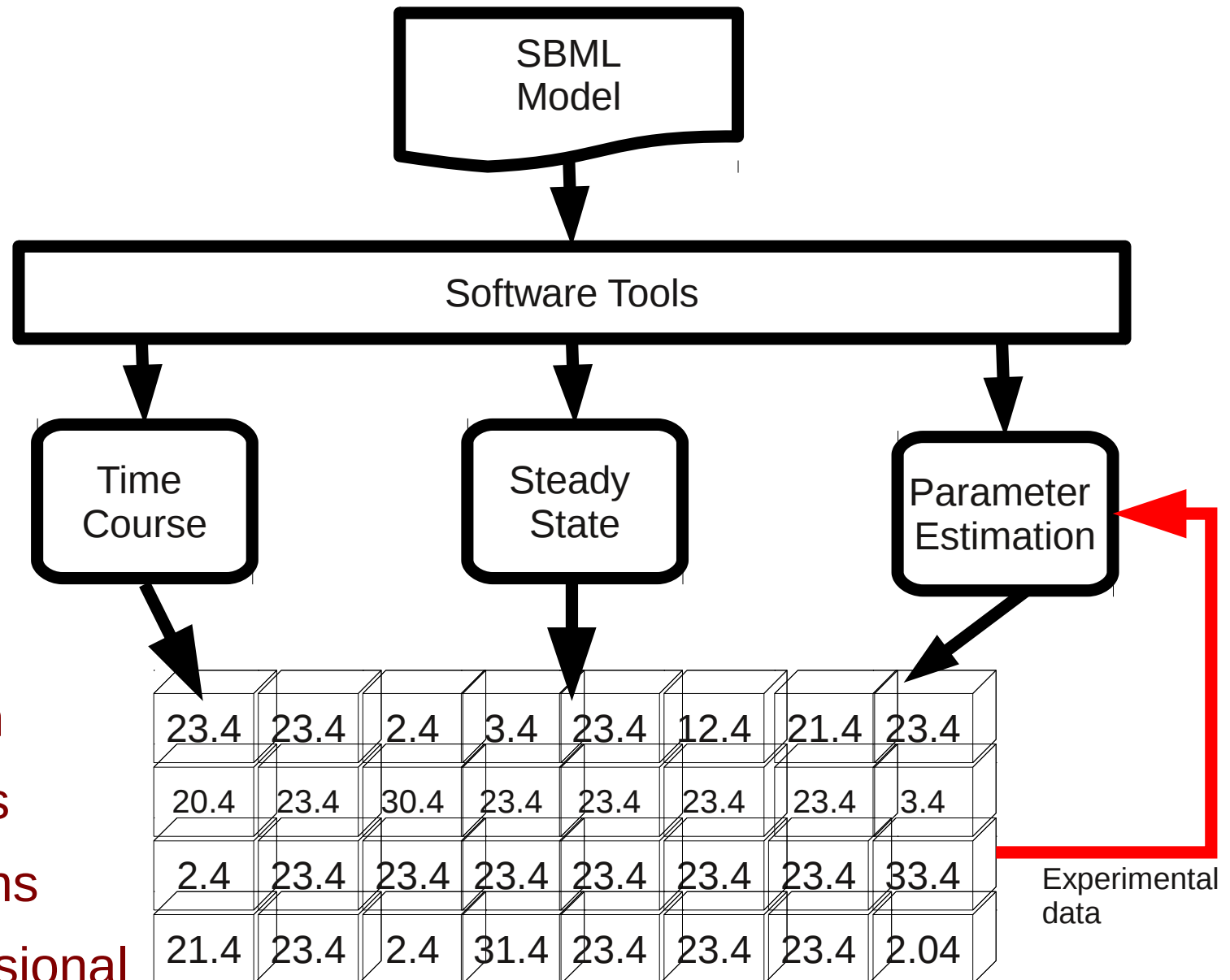
Associate Editor: Trey Ideker

- Meeting in ICSB conf/SBML Forum in Heiderberg 2011
- Adopted as data encoding format for SED-ML in Harmony 2013

Aims of NuML

- To standardize the exchange of numerical results
- Re-use in multiple other standardization efforts
- Parsing experimental data to simulators
- Recording the results of analysis for validation and analysis

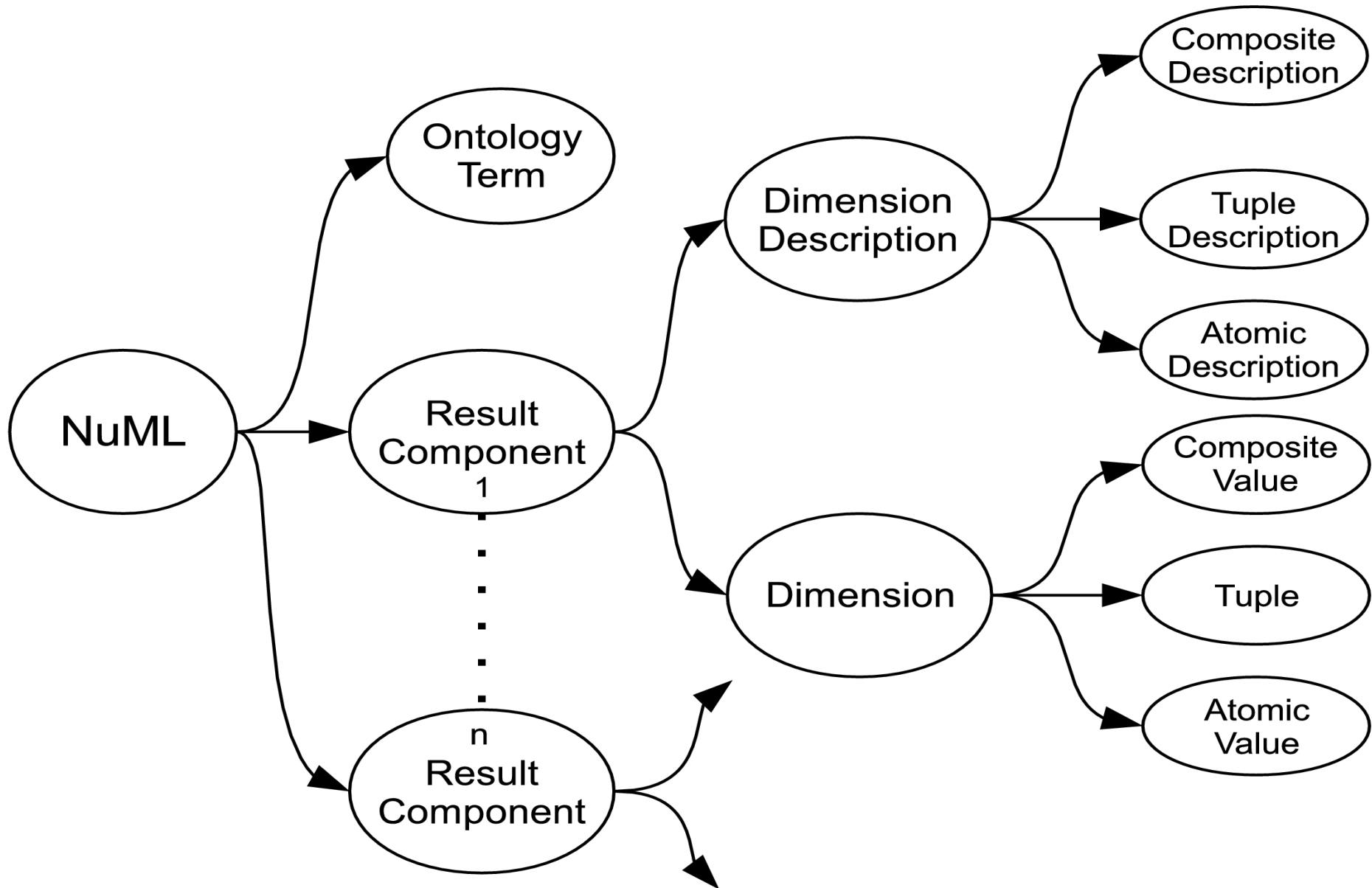
Examples of Numerical Results



- Data

- Simple
- 1 dimension
- 2 Dimensions
- 3 Dimensions
- Multi-dimensional

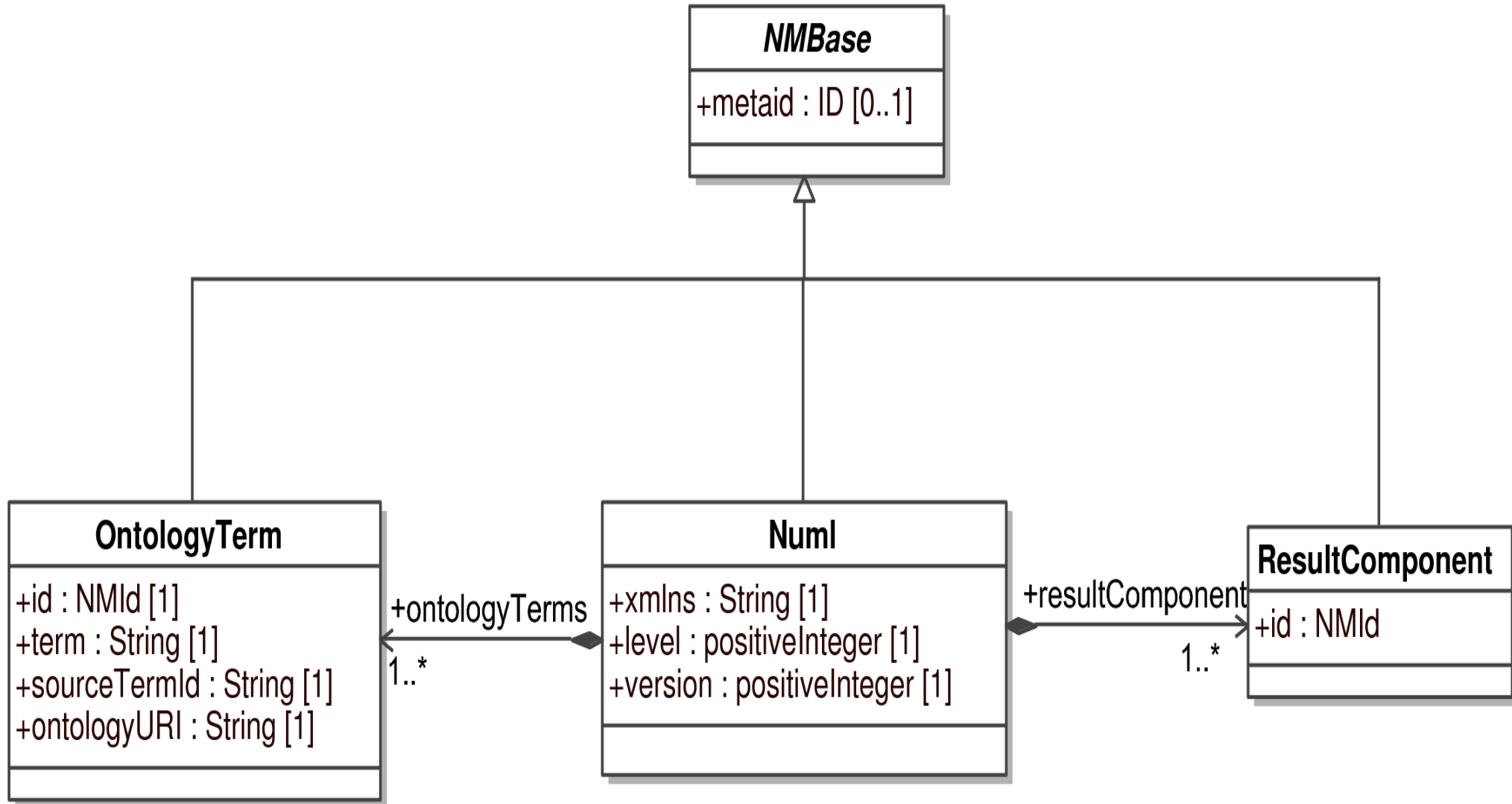
Overview of NuML



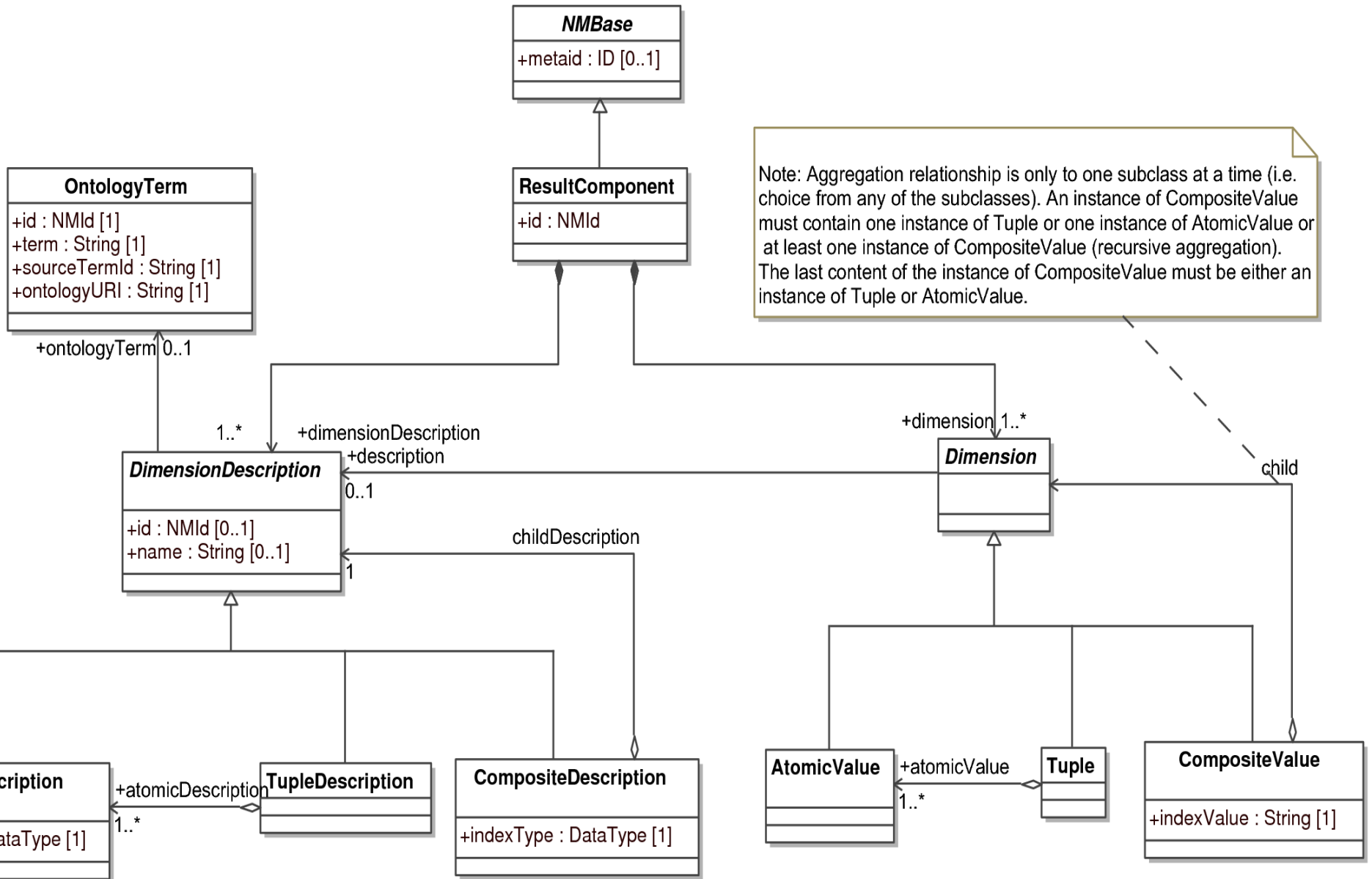
Specification

- Specification Level 1 Version 1
 - <http://code.google.com/p/numl/source/browse/trunk/numl-spec-l1v1.pdf>
- UML Model
- XML Schema

NuML Object Model



Result Component Object Model



NuML Document Example

```
<?xml version="1.0" encoding="UTF-8"?>
<numl version="1" level="1" xmlns="http://www.numl.org/numl/level1/version1">
  <ontologyTerms>
    <ontologyTerm id="term1" term="time" sourceTermId="SBO:0000345" ontologyURI="http://www.ebi.ac.uk/sbo/" />
    <ontologyTerm id="term2" term="concentration" sourceTermId="SBO:0000196" ontologyURI="http://www.ebi.ac.uk/sbo/" />
  </ontologyTerms>
  <resultComponent id="component1">
    <dimensionDescription>
      <compositeDescription name="Time" ontologyTerm="term1" indexType="double">
        <compositeDescription name="Species" indexType="xpath">
          <atomicDescription name="Concentration" ontologyTerm="term2" valueType="double" />
        </compositeDescription>
      </compositeDescription>
    </dimensionDescription>
    <dimension>
      <compositeValue indexValue="0">
        <compositeValue indexValue="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='x_CO2']">
          <atomicValue>1</atomicValue>
        </compositeValue>
        <compositeValue indexValue="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='RuBP_ch']">
          <atomicValue>0.33644</atomicValue>
        </compositeValue>
        <compositeValue indexValue="/sbml:sbml/sbml:model/sbml:listOfSpecies/sbml:species[@id='PGA_ch']">
          <atomicValue>3.35479</atomicValue>
        </compositeValue>
      </compositeValue>
    </dimension>
  </resultComponent>
  <resultComponent id="recomponet2"> ... </resultComponent>
</numl>
```

```

<resultComponent id="species_conc">
  <dimensionDescription>
    <compositeDescription name="Time" ontologyTerm="term3" indexType="float">
      <compositeDescription name="Metabolite" ontologyTerm="term2" indexType="string">
        <atomicDescription name="Concentration" ontologyTerm="term1" valueType="double" />
      </compositeDescription>
    </compositeDescription>
  </dimensionDescription>
  <dimension>
    <compositeValue indexValue="0">
      <compositeValue indexValue="BL">
        <atomicValue>0.0</atomicValue>
      </compositeValue>
    </compositeValue>
    <compositeValue indexValue="1">
      <atomicValue>1.66058</atomicValue>
    </compositeValue>
    <compositeValue indexValue="DLL">
      <atomicValue>8.84913e-2</atomicValue>
    </compositeValue>
  </dimension>
  <compositeValue indexValue="20">
    <compositeValue indexValue="BL">
      <atomicValue>0.23</atomicValue>
    </compositeValue>
    <compositeValue indexValue="B">
      <atomicValue>1.76058</atomicValue>
    </compositeValue>
    <compositeValue indexValue="DLL">
      <atomicValue>9.84913e-2</atomicValue>
    </compositeValue>
  </compositeValue>
</dimension>
</resultComponent>

```

Time Course Data

```

<resultComponent id="species_con_pnumbers">
  <dimensionDescription>
    <compositeDescription name="species" indexType="string">
      <tupleDescription>
        <atomicDescription name="Concentration" ontologyTerm="term1" valueType="double" />
        <atomicDescription name="Particle Numbers" ontologyTerm="term2" valueType="double" />
      </tupleDescription>
    </compositeDescription>
  </dimensionDescription>
  <dimension>
    <compositeValue indexValue="PhosId">
      <tuple>
        <atomicValue>141.063</atomicValue>
        <atomicValue>8.49503e+19</atomicValue>
      </tuple>
    </compositeValue>
    <compositeValue indexValue="InphosId">
      <tuple>
        <atomicValue>12000</atomicValue>
        <atomicValue>6.02214e+21</atomicValue>
      </tuple>
    </compositeValue>
    <compositeValue indexValue="CysId">
      <tuple>
        <atomicValue>150.034</atomicValue>
        <atomicValue>9.03321e+18</atomicValue>
      </tuple>
    </compositeValue>
  </dimension>
</resultComponent>

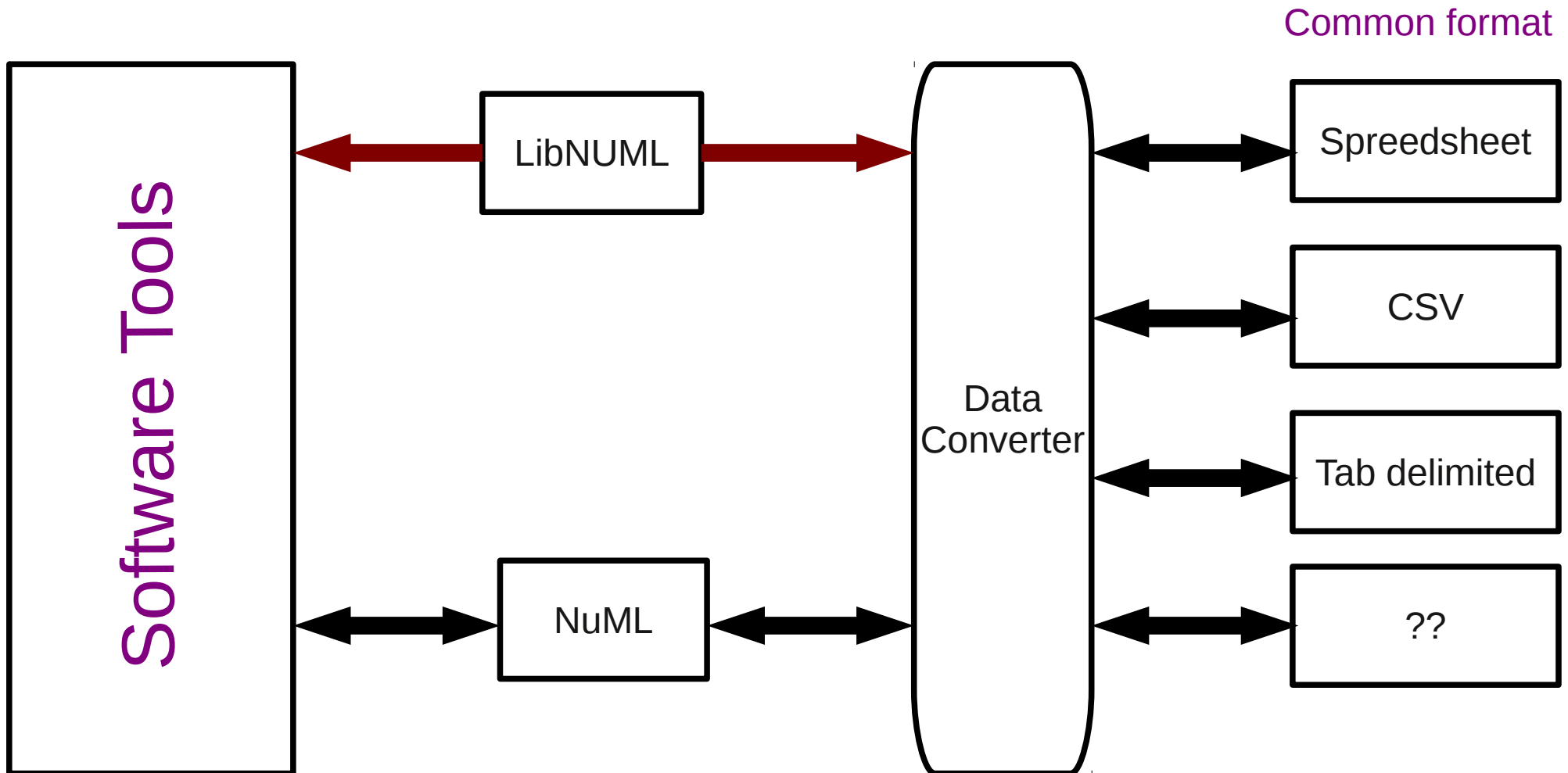
```

Species concentration & Particle Numbers

LibNUML

- Library for reading, writing and manipulating data in NuML on all operating systems
- Develop in C/C++ language
 - Can be compiled on different operating systems
- Bindings in Java and Python languages
- Other language bindings on demand
- Examples in C/C++ and bindings

Data Converter



Expected NuML Tools

- Data Converter
 - Conversion of common data format to NuML
- Generator
 - Generation of NuML data from simulated SBML model
- Validator
 - Validation of NuML document
- Online Web Tools

Links to Resources

- Code base
 - <http://code.google.com/p/numl/>
- Specification level 1 version 1
 - <http://code.google.com/p/numl/source/browse/trunk/numl-spec-l1v1.pdf>
- Schema
 - <http://code.google.com/p/numl/source/browse/trunk/NUMLSchema.xsd>
- LibNUMML
 - <http://numl.googlecode.com/svn/trunk/libnuml/>
- Mailing list
 - <http://groups.google.com/group/numl-discuss/>

Thanks & Questions