NuML: Numerical Markup Language
&
LibNUML

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Origin 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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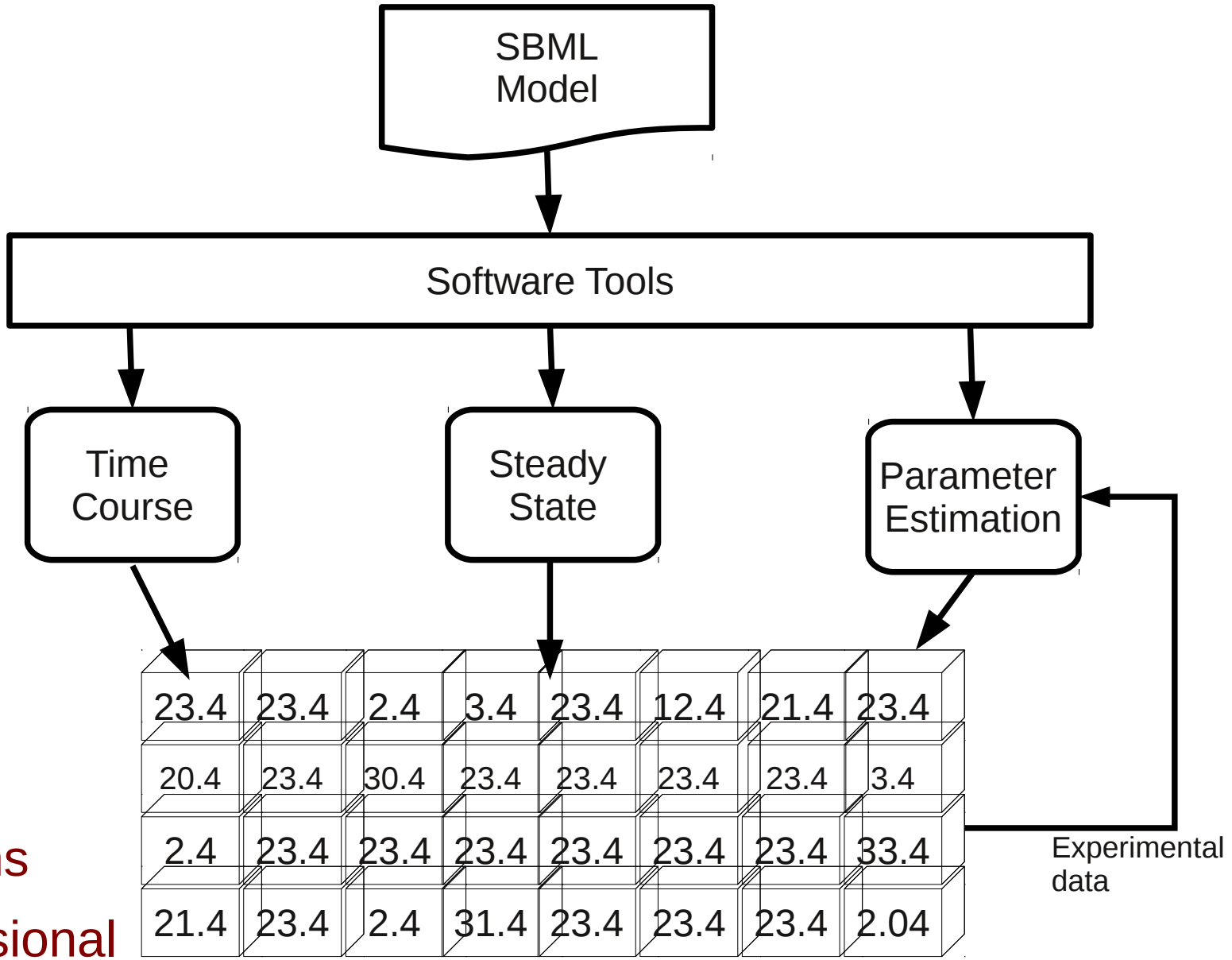
- Idea from meeting in ICSB conf/SBML Forum in Heiderberg
  - Pedro Mendes, Joseph O. Dada, Sven Sahle, Frank Bergmann & Nicolas Le Novere
  - Meeting outcome presented to the SBML forum by Frank

XML Language for Ecoding Numerical Results

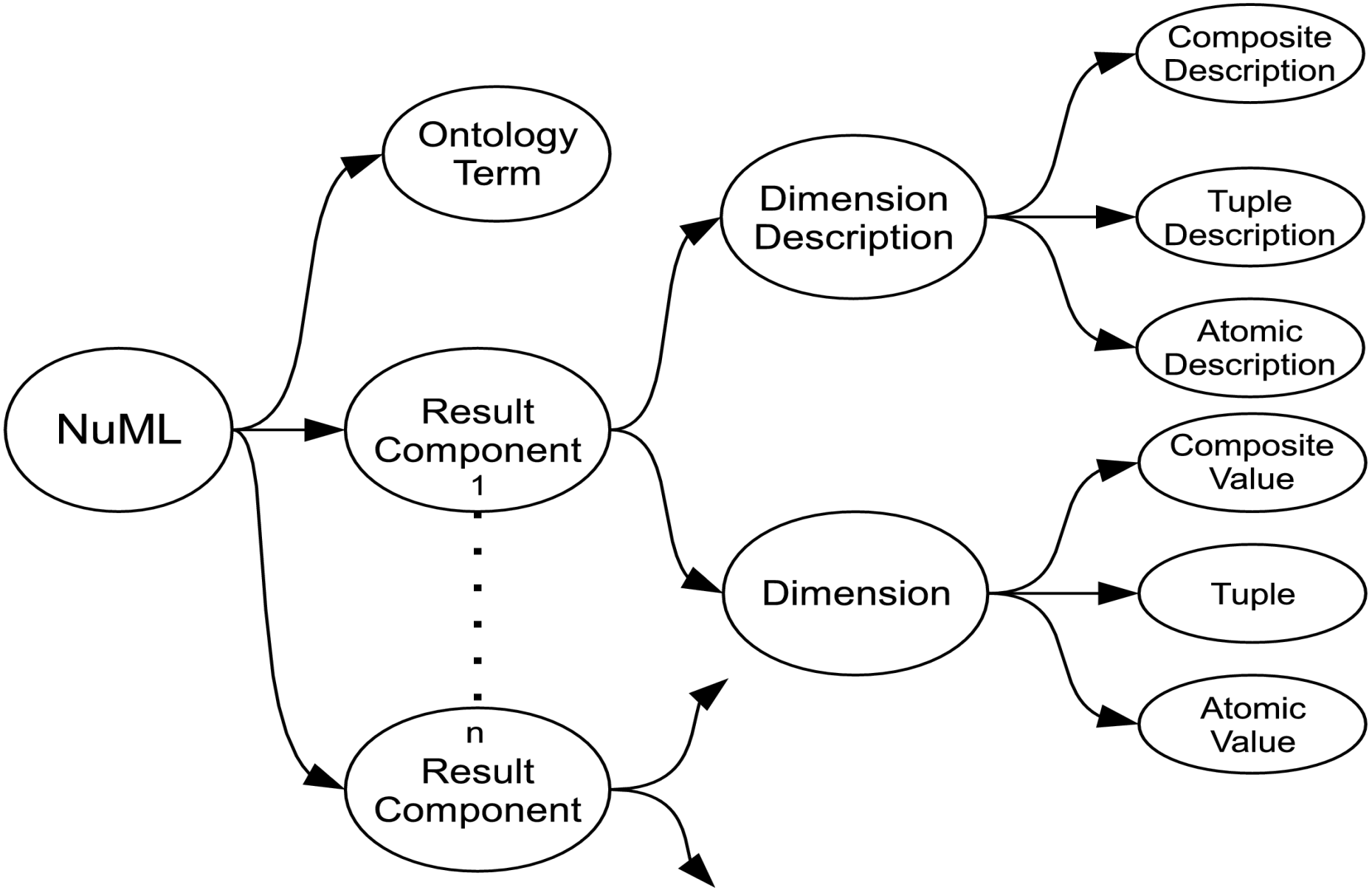
- Data
  - Simple
  - 1 dimension
  - 2 Dimesions
  - 3 Dimensions
  - Multi-dimensional



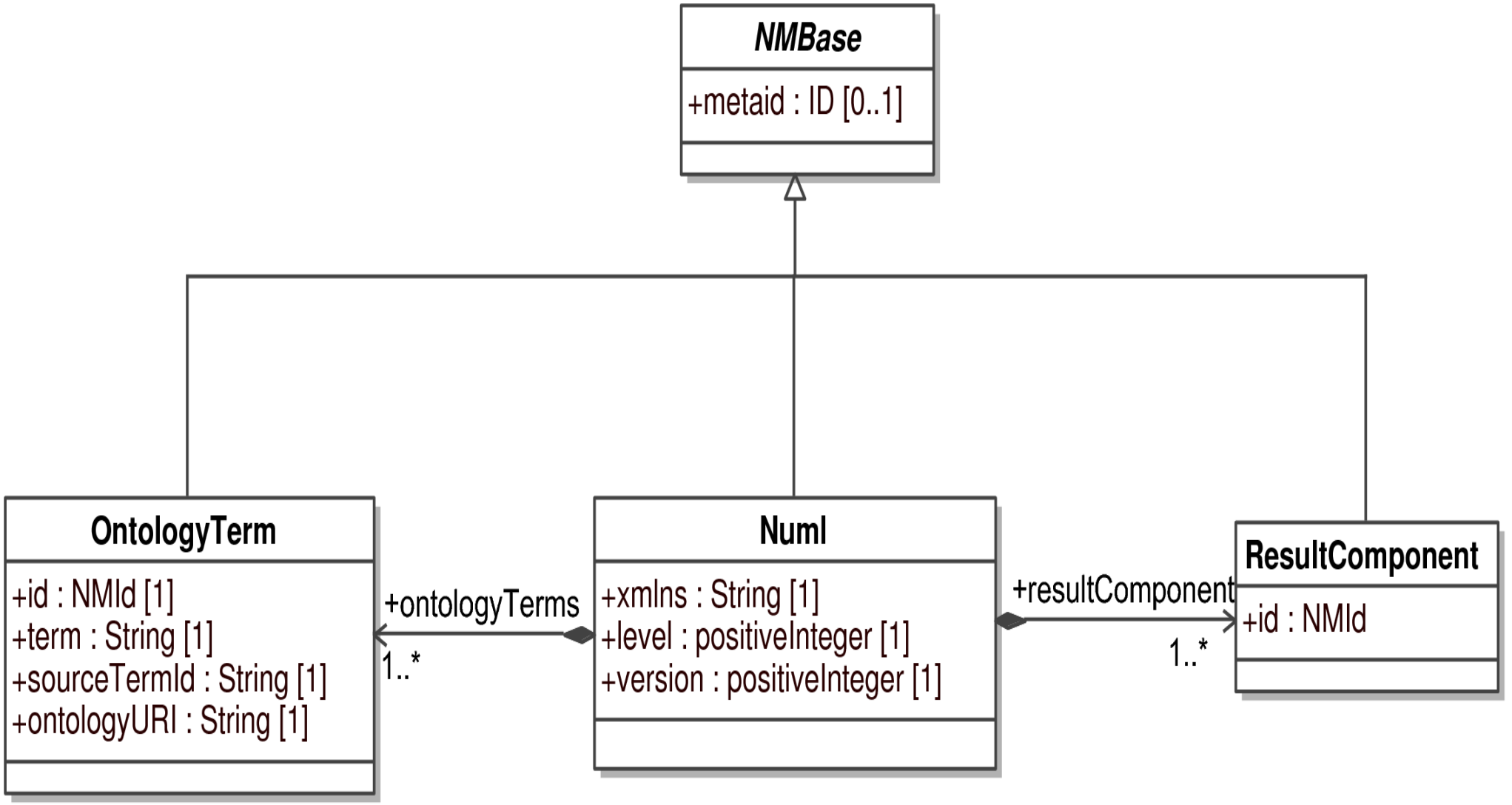
Aims of NuML

- Provide a flexible and powerful structure for encoding numerical data
- 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
- ??

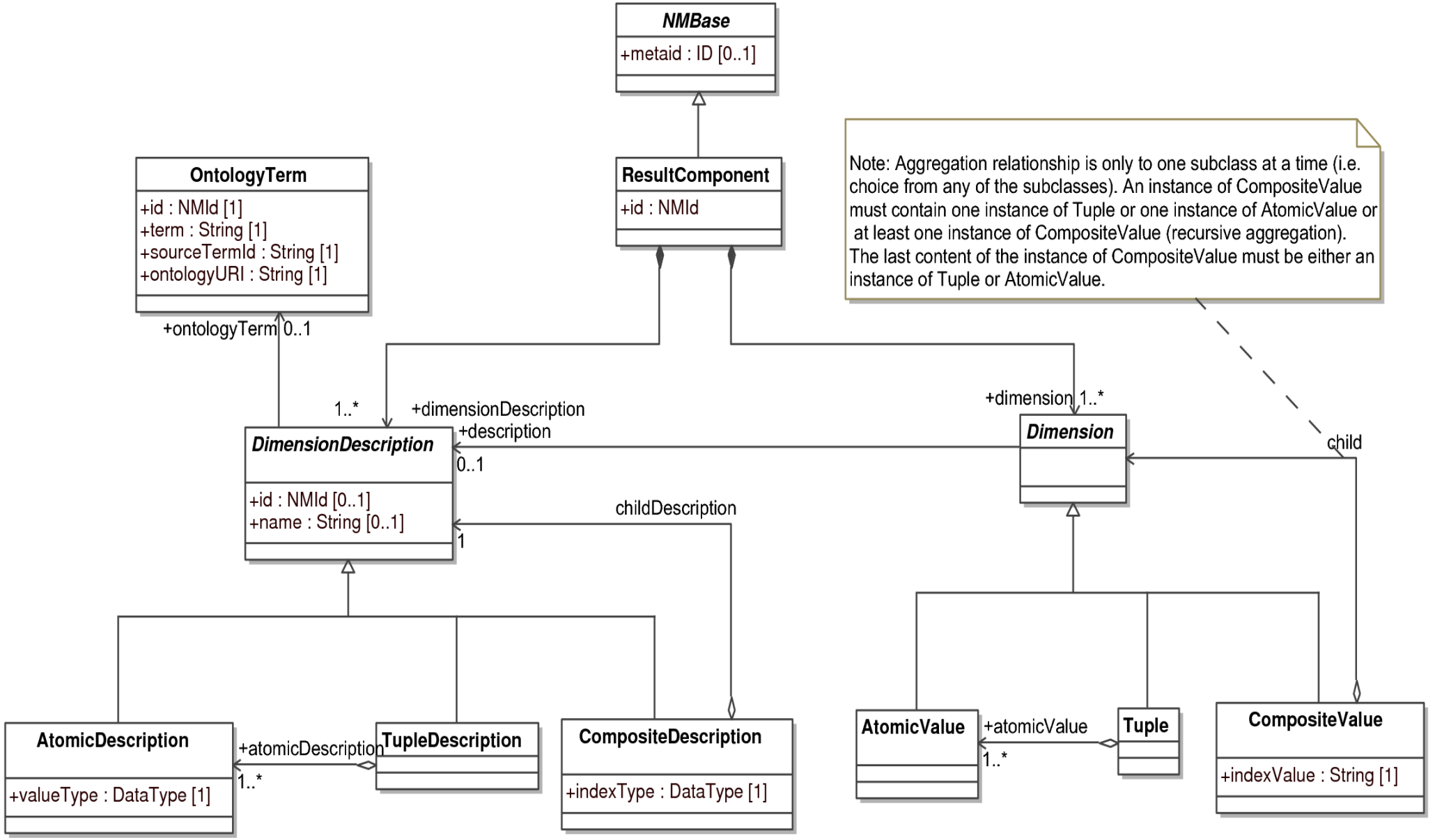
Overview of NuML



NuML Object Model



NuML Complete 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>
```

```
<resultComponents>
  <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 indexValue="B">
     <atomicValue>1.66058</atomicValue>
   </compositeValue>
   <compositeValue indexValue="DLL">
     <atomicValue>8.84913e-2</atomicValue>
    </compositeValue>
  </compositeValue>
  <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>
</resultComponents>
```

Time Course Data

Time	BL	B	DLL
0	0.0	1.66058	8.84913e-2
20	0.23	1.76058	9.84913e-2
40	..	..	...

```
<resultComponents>
  <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>
</resultComponents>
```

Species concentration & Particle Numbers

Species	Concentration	Particle Numbers
PhosId	141.063	8.49503e+19
InphosId	12000	6.02214e+21
CysId	150.034	9.03321e+18

LibNUML

- Library for reading, writing and manipulating data in NuML on all operating systems
- Develop C/C++ library
  - Can be compiled on different operating systems
- Use XML parser layer of libSBML
- Easy consistency and validity checking
- Bindings in other major languages
  - Java available, C#, pathon, etc to follow
- Examples in C/C++ and binding languages

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
- LibNUML
  - http://numl.googlecode.com/svn/trunk/libnuml/
- Mailing list
  - http://groups.google.com/group/numl-discuss/

Thanks!