

Systems Biology Results Markup Language (SBRML)

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Outline

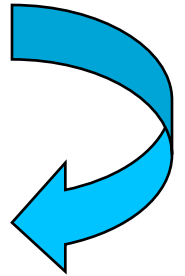
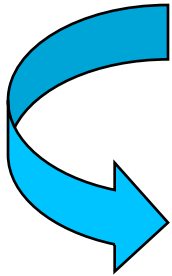
- Introduction & Motivation
- The SBRML
 - What is SBRML?
 - Overview of SBRML
 - SBRML UML Model & Examples
- Online Examples
- Conclusions & Future Plans

Introduction & Motivation

- SBML
 - *De facto* standard for specifying models of biochemical systems
 - Supported by many software vendors
 - Many models are now in electronic format
- Many other standardization activities
 - MIRIAM
 - SBGN
 - MIASE
 - Ontology
 - SBO
 - KiSAO

Introduction & Motivation

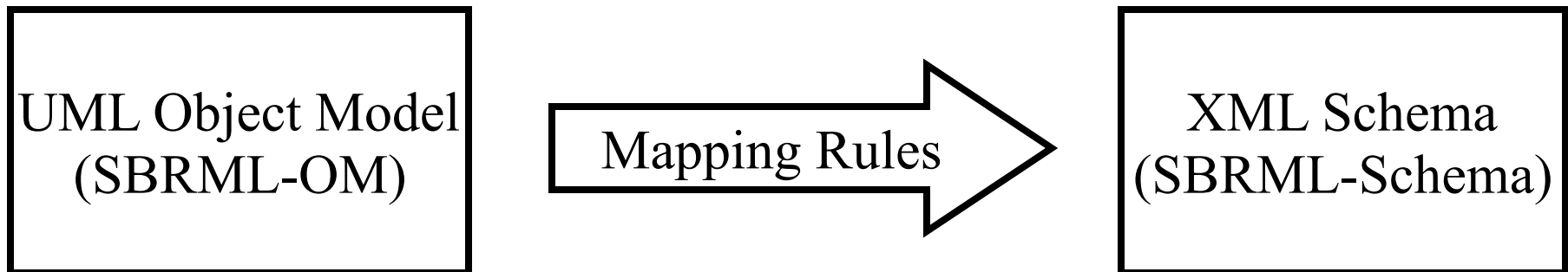
- Currently no standard way for communicating the results of operation carried out on SBML models



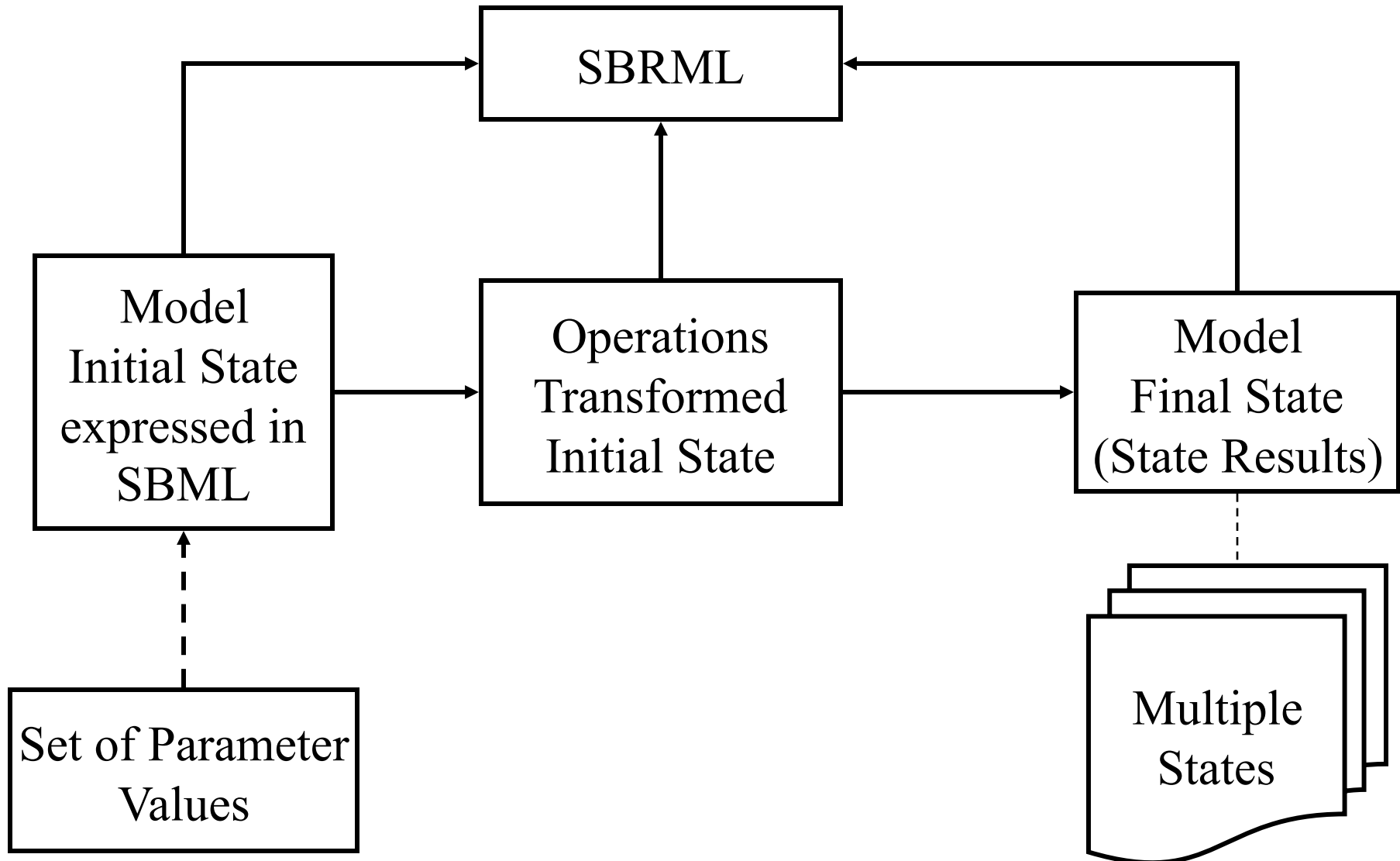
Systems biology community needs a good representation to communicate the results of operation done with SBML models

What is SBRML?

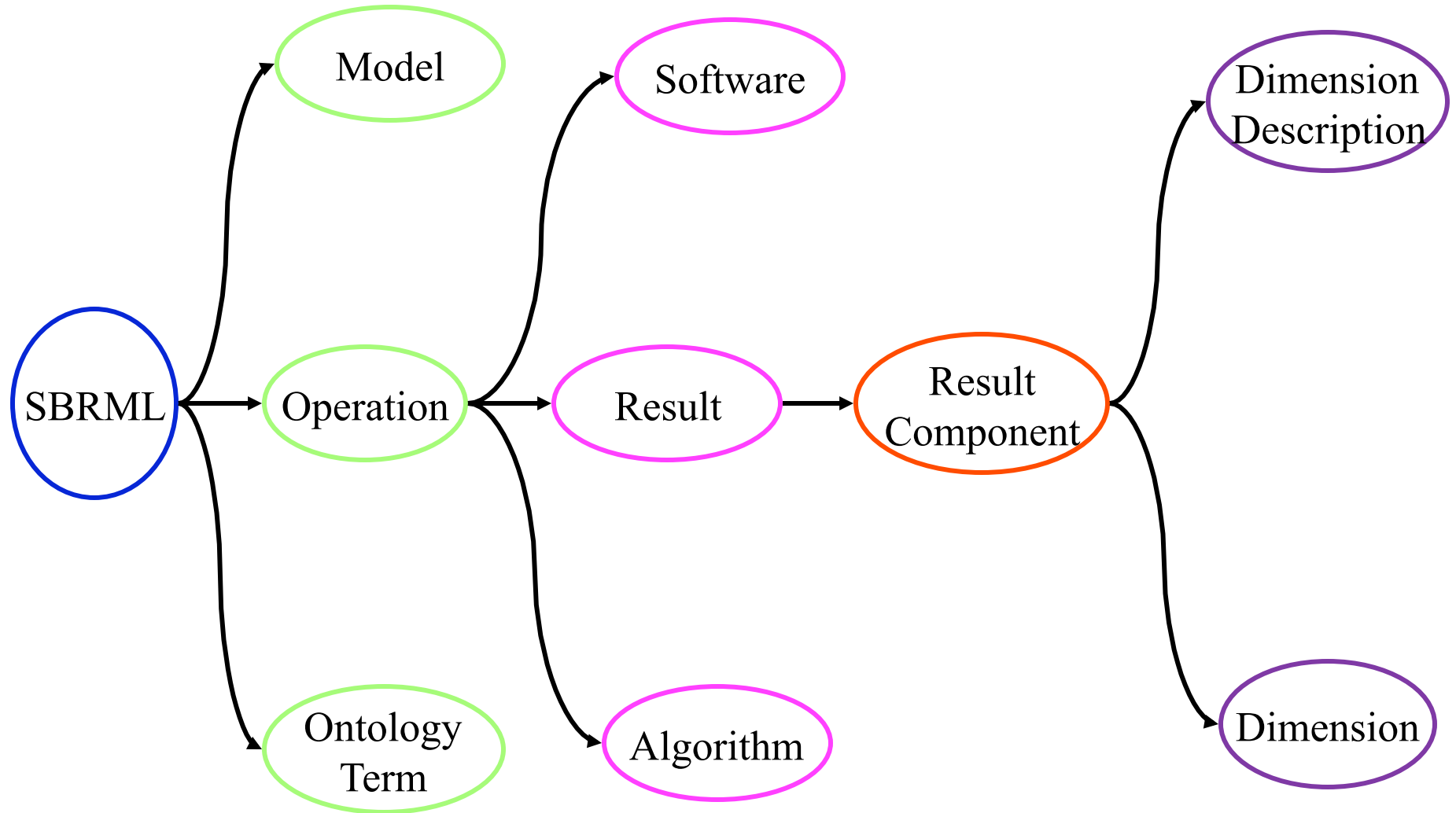
- A new markup language for specifying the results from operations on SBML models
- Useful to communicate experimental data



Overview of SBRML



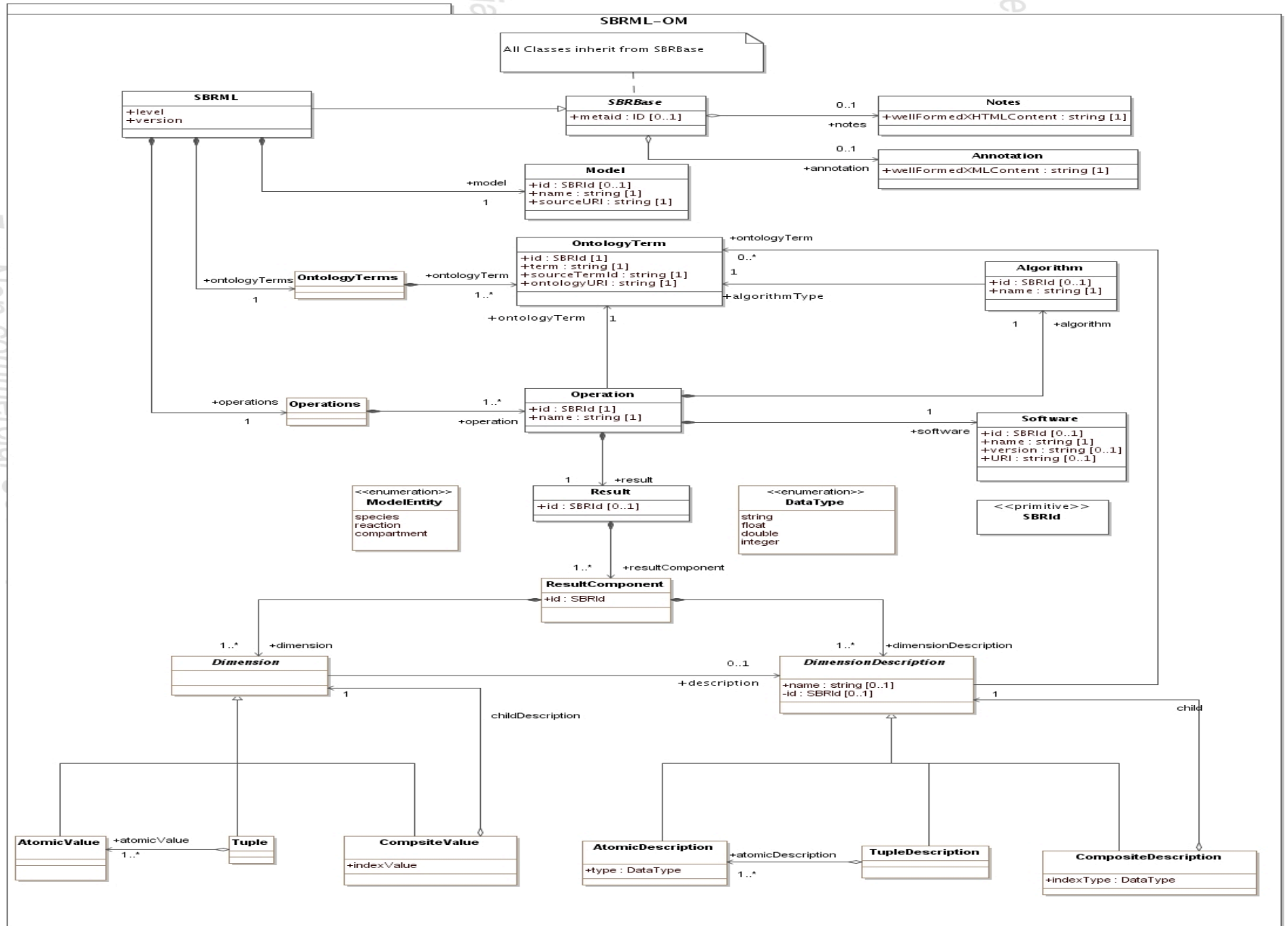
Overview of SBRML



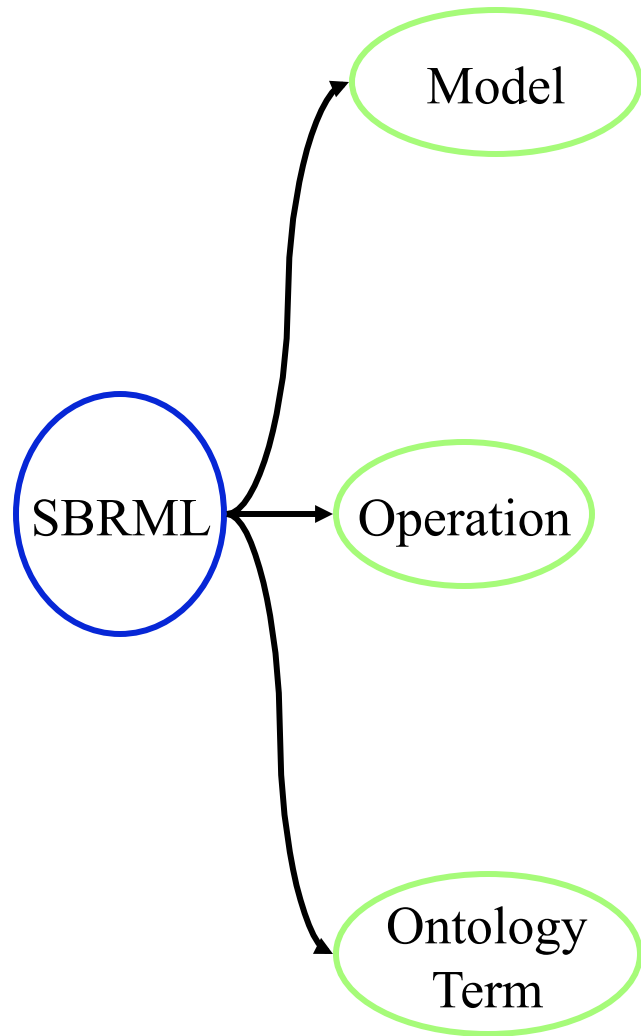
- Results can be encoded as
 - Tuples
 - Multidimensional data

SBRML UML Model & Examples

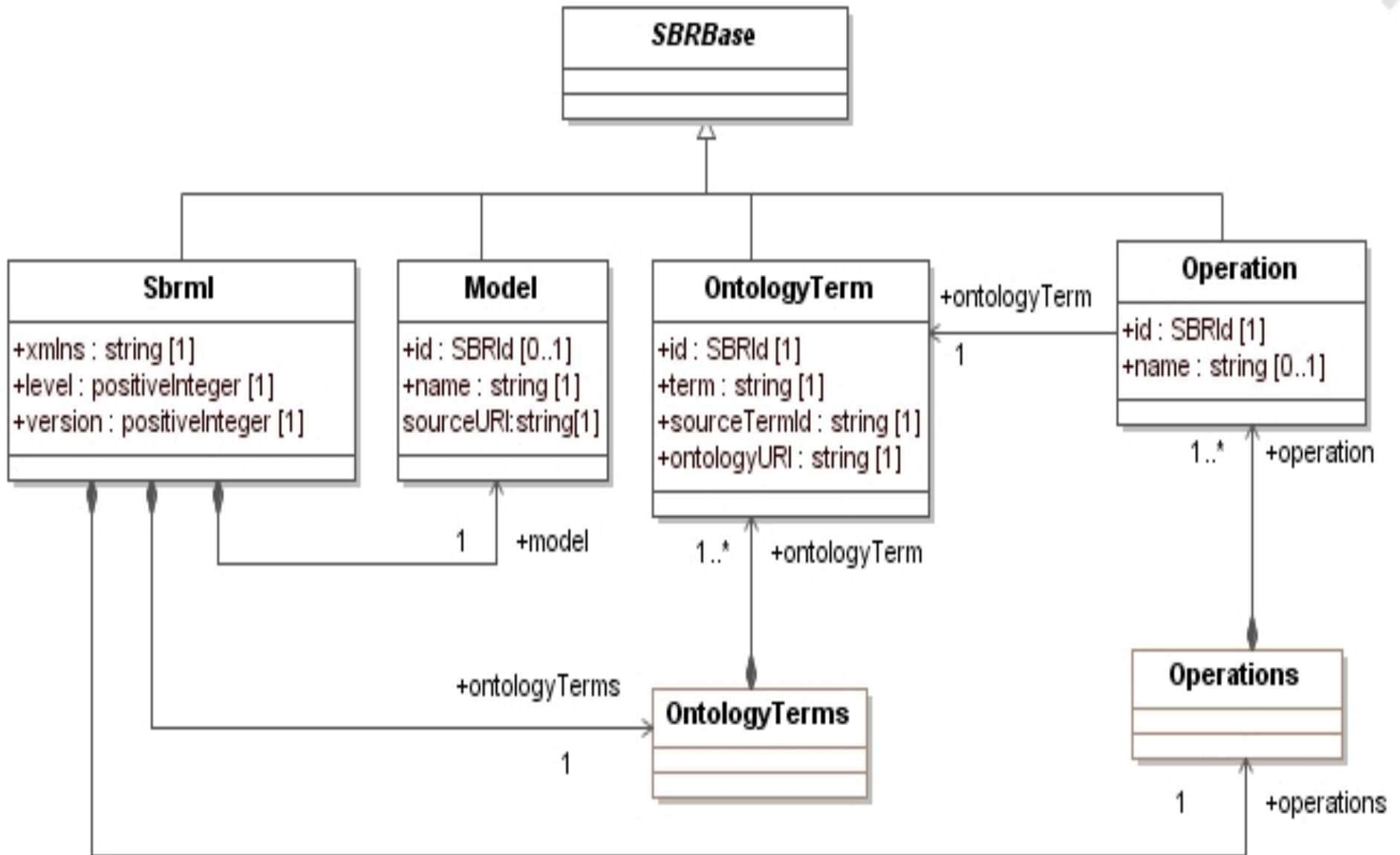
SBRML-OM



Overview of SBRML



SBRML Top Level Object Model



SBRML Example

```
<?xml version="1.0" encoding="UTF-8"?>
```

```
<sbrml xmlns="http://www.comp-sys-bio.org/sbrml/level1" version="1.0"  
level="1.0">
```

```
<ontologyTerms>
```

```
  <ontologyTerm id="term1" term="Steady State"  
sourceTermId="Term00001" ontologyURI="TestOntoWebSite.org" />
```

```
</ontologyTerms>
```

```
<model id="model1" name="Edelstein1996_.." sourceURI="file://BIO..1" />
```

```
<operations>
```

```
  <operation id="op1" ontologyTerm="term1">
```

```
    ...
```

```
  </operation>
```

```
</operations>
```

```
</sbrml>
```

OntologyTerms Example

```
<ontologyTerms>
```

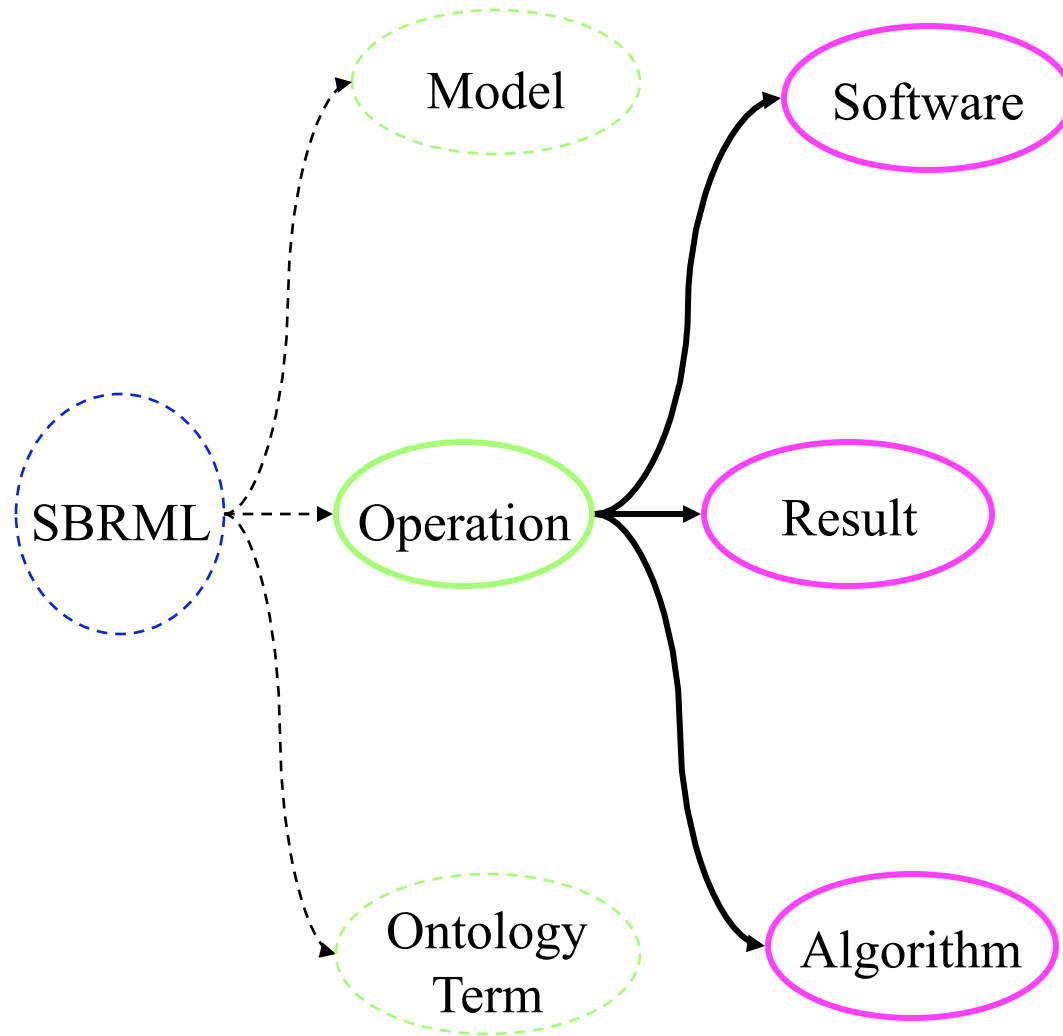
```
  <ontologyTerm id="term1" term="Steady State"  
  sourceTermId="Term00001" ontologyURI="TestOntoWebSite.org" />
```

```
  <ontologyTerm id="term2" term="Euler method"  
  sourceTermId="KISAO:0000030" ontologyURI="http://www.ebi./  
kisao/" />
```

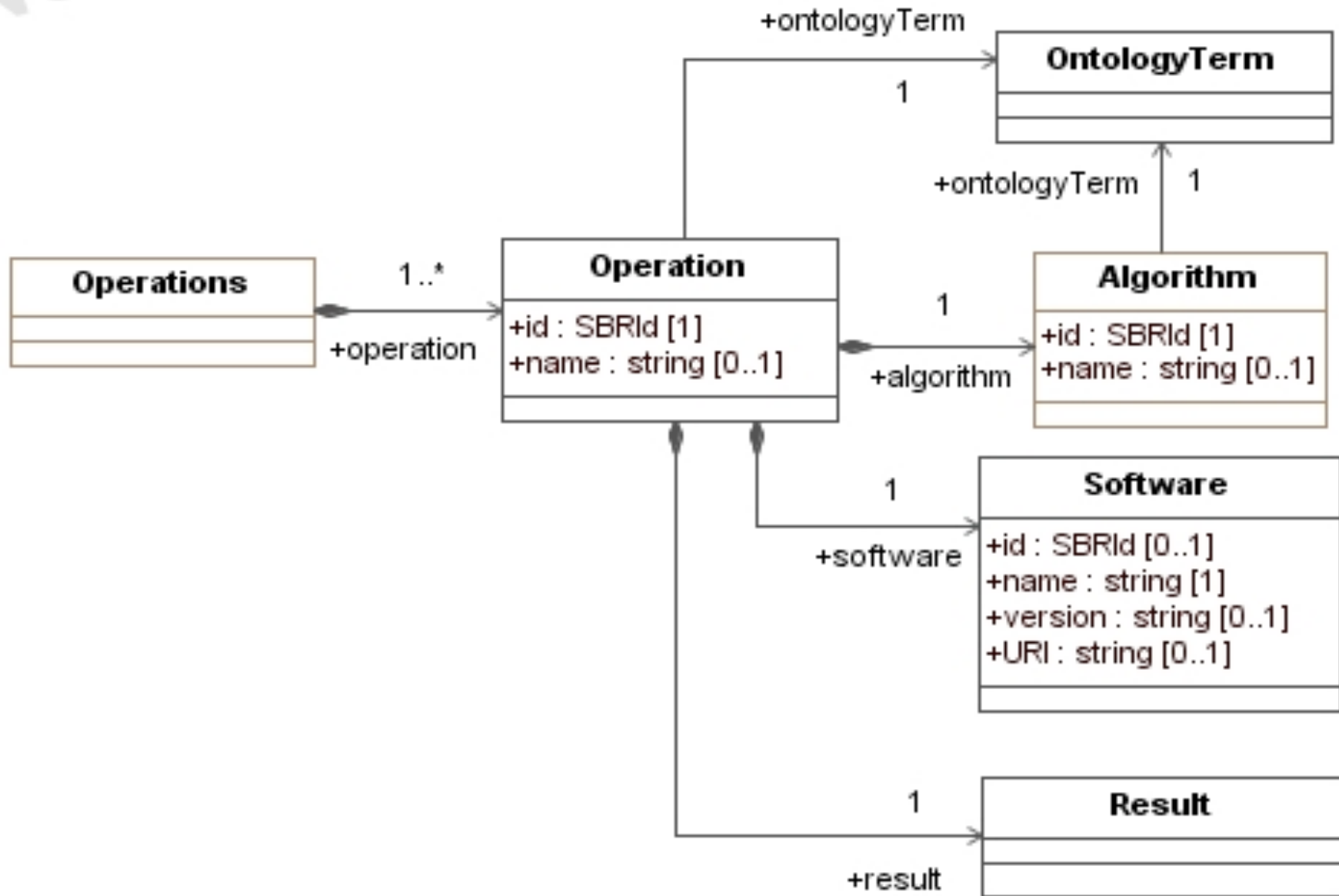
```
  <ontologyTerm id="term3" term="concentration" sourceTermId="SBO:  
0000196" ontologyURI="http://www.ebi.ac.uk/sbo/" />
```

```
</ontologyTerms>
```

Overview of SBRML



Operation Object Model



Operation Example

```
<operations>
```

```
<operation id="op1" ontologyTerm="term1">
```

```
<algorithm id="algo1" ontologyTerm="term2" />
```

```
<software id="soft1" name=" COPASI" version="COPASI 4.4  
Build 26" URI="http://www.copasi.org" />
```

```
<result>
```

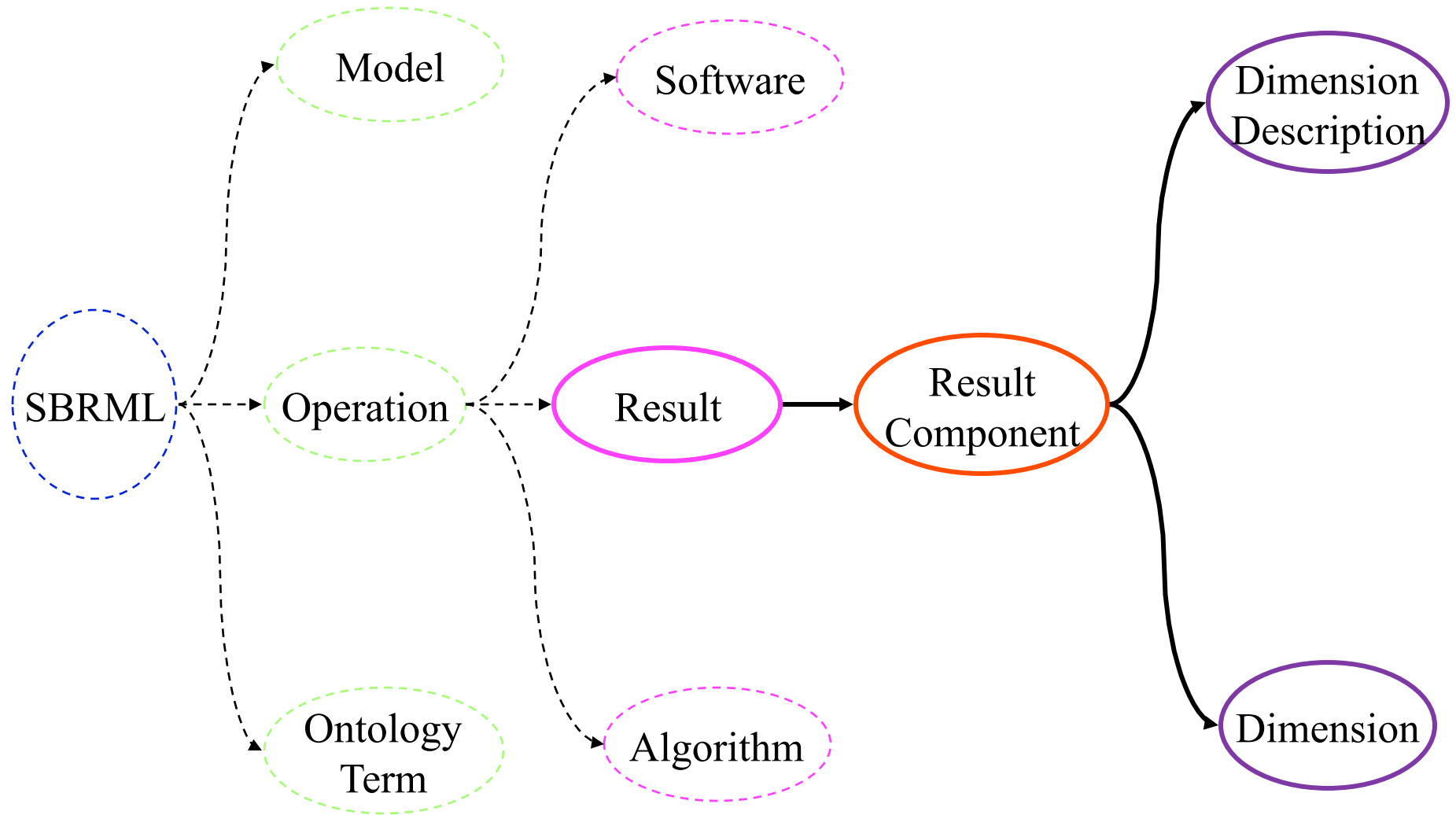
```
...
```

```
</result>
```

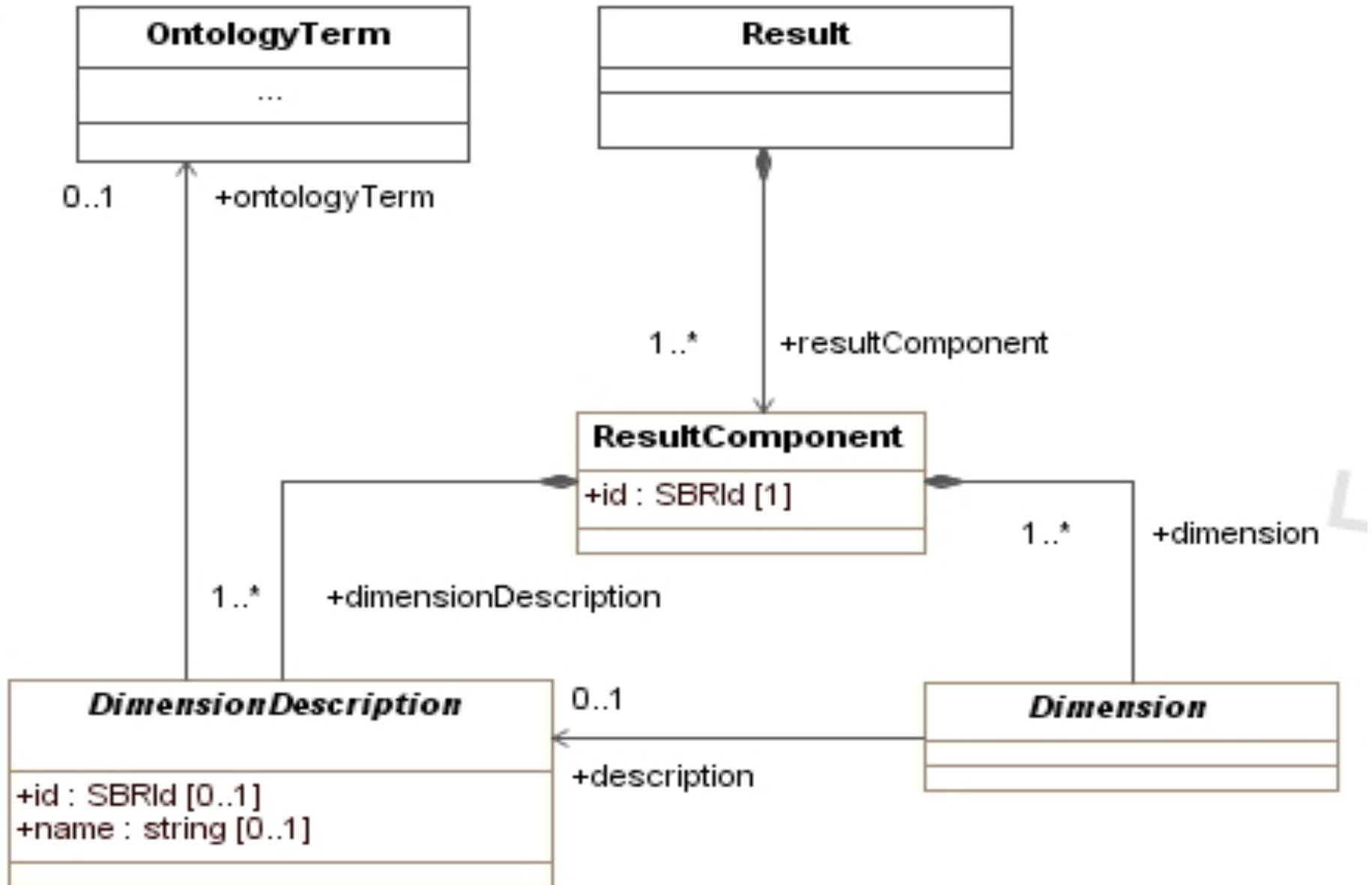
```
</operation>
```

```
</operations>
```

Overview of SBRML



Result (Component) Object Model



Result (Component) Example

<result>

<resultComponent id="component11">

<dimensionDescription>

...

</dimensionDescription>

<dimension>

...

<dimension>

</resultComponent>

<resultComponent id="component12">

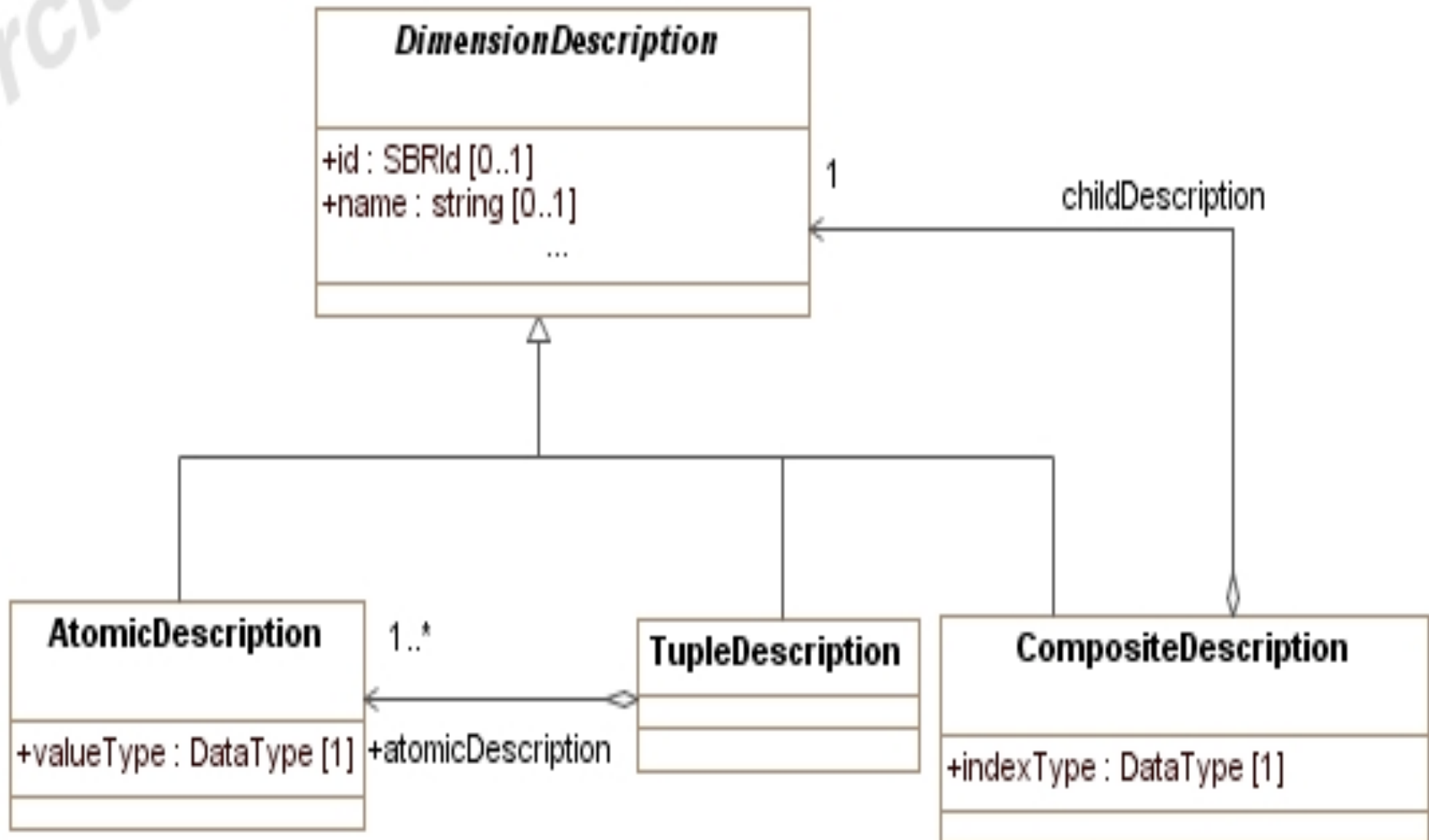
...

...

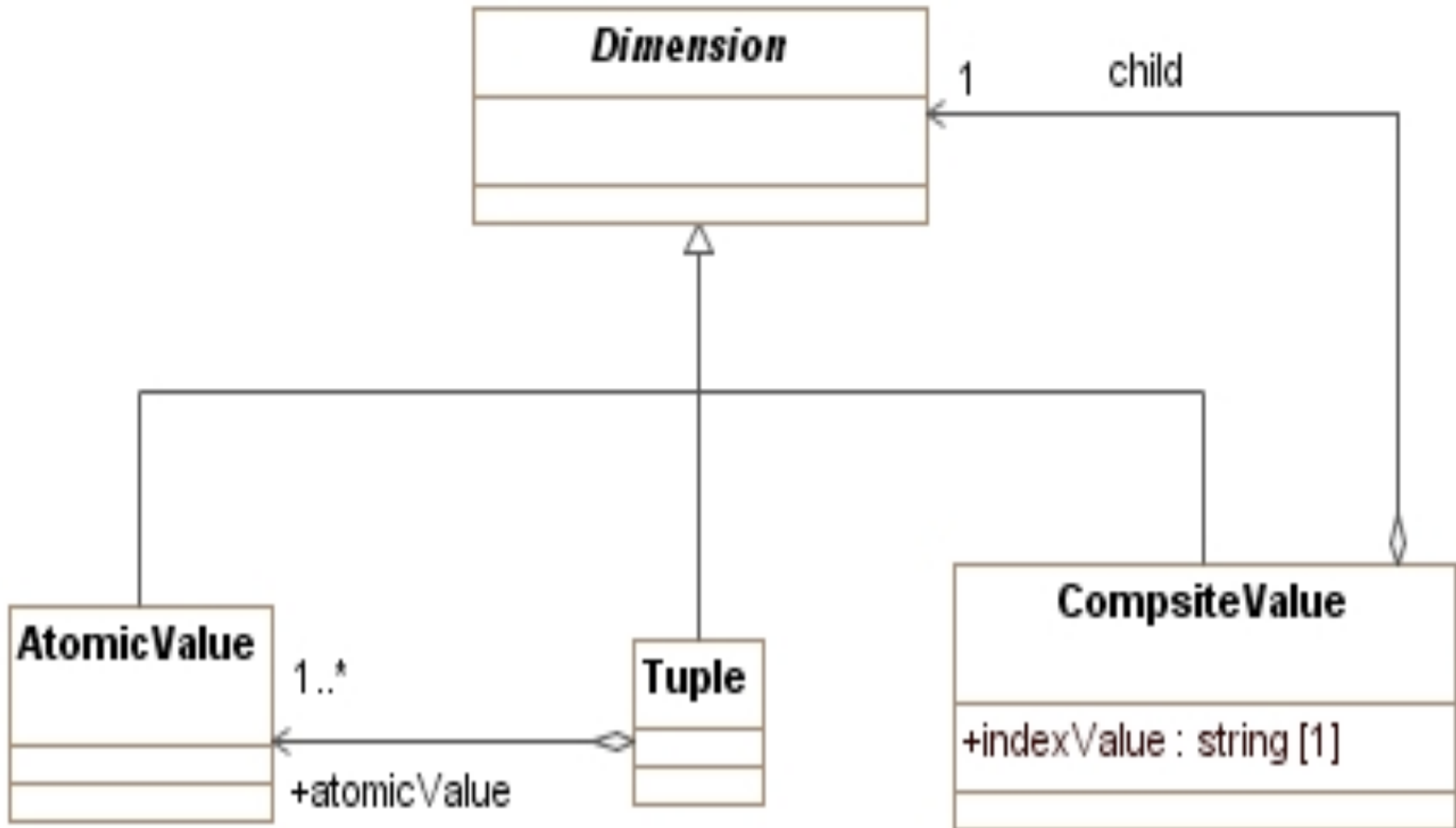
</resultComponent>

</result

Dimension Description Object Model



Dimension



Dimension Description Example

```
<dimensionDescription>
```

```
  <compositeDescription name="Species" ontologyTerm="term5"  
  indexType="string">
```

```
    <tupleDescription>
```

```
      <atomicDescription name="Concentration" ontologyTerm="term3"  
      valueType="double" />
```

```
      <atomicDescription name="Particle Numbers"  
                          ontologyTerm="term4" valueType="double" />
```

```
    </tupleDescription>
```

```
  </compositeDescription>
```

```
</dimensionDescription>
```

Dimension Example

<dimension>

<compositeValue indexValue="Basal">

<tuple>

<atomicValue>1.66058e-05</atomicValue>

<atomicValue>1000.02</atomicValue>

</tuple>

</compositeValue>

<compositeValue indexValue="DesensitisedACh2">

<tuple>

<atomicValue>8.84913e-23</atomicValue>

<atomicValue>5.32907e-15</atomicValue>

</tuple>

</compositeValue>

</dimension>

Online Examples

<http://garfinkel.mib.man.ac.uk:8080/CopasiWeb/CopasiWebUI>



- [Home](#)
- [Services Home](#)
- [COPASI Home](#)

Steady State Web Services

SBML File:

Available Services

- Model Processor
 - [SBML To Copasi ML](#)
 - [Copasi ML To SBML](#)
 - [Validate Model](#)
- Steady State
 - Synchronous Model
 - [Copasi ML](#)
 - [SBML](#)
 - Asynchronous Model
 - [Copasi ML](#)
 - [SBML](#)

Choose file

Look in: curated

BIOMD0000000001	BIOMD0000000016	BIOMD0000000032	BIOMD0000000048
BIOMD0000000002	BIOMD0000000017	BIOMD0000000033	BIOMD0000000049
BIOMD0000000003	BIOMD0000000018	BIOMD0000000034	BIOMD0000000050
BIOMD0000000004	BIOMD0000000019	BIOMD0000000035	BIOMD0000000051
BIOMD0000000005	BIOMD0000000020	BIOMD0000000036	BIOMD0000000052
BIOMD0000000006	BIOMD0000000021	BIOMD0000000037	BIOMD0000000053
BIOMD0000000007	BIOMD0000000022	BIOMD0000000038	BIOMD0000000054
BIOMD0000000008	BIOMD0000000023	BIOMD0000000039	BIOMD0000000055
BIOMD0000000009	BIOMD0000000024	BIOMD0000000040	BIOMD0000000056
BIOMD0000000010	BIOMD0000000025	BIOMD0000000041	BIOMD0000000057
BIOMD0000000011	BIOMD0000000026	BIOMD0000000042	BIOMD0000000058
BIOMD0000000012	BIOMD0000000027	BIOMD0000000043	BIOMD0000000059
BIOMD0000000013	BIOMD0000000028	BIOMD0000000044	BIOMD0000000060
BIOMD0000000014	BIOMD0000000029	BIOMD0000000045	BIOMD0000000061
BIOMD0000000015	BIOMD0000000030	BIOMD0000000046	BIOMD0000000062
BIOMD0000000016	BIOMD0000000031	BIOMD0000000047	BIOMD0000000063

File name: BIOMD0000000001

Files of type: All Files (*.*)



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- [Home](#)
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Available Services

- Model Processor
 - [SBML To Copasi ML](#)
 - [Copasi ML To SBML](#)
 - [Validate Model](#)
- Steady State
 - Synchronous
 - Model
 - [Copasi ML](#)
 - [SBML](#)
 - Asynchronous
 - Model
 - [Copasi ML](#)
 - [SBML](#)

```
<?xml version="1.0" encoding="UTF-8" ?>
- <sbml xmlns="http://www.sbml.org/sbml/level1" version="1.0" level="1.0">
- <ontologyTerms>
  <ontologyTerm id="term1" term="Enhanced Newton" sourceTermId="" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term2" term="Steady State" sourceTermId="" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term3" term="concentration" sourceTermId="SBO:0000196" ontologyURI="http://www.ebi.ac.uk/sbo/" />
  <ontologyTerm id="term4" term="particel numbers" sourceTermId="TestId:0000008" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="terms5" term="species" sourceTermId="TestId:0000007" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term6" term="reaction" sourceTermId="TestId:0000009" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term7" term="flux" sourceTermId="TestId:0000010" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term8" term="particle flux" sourceTermId="TestId:0000011" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term9" term="compartment" sourceTermId="TestId:0000012" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term10" term="size" sourceTermId="TestId:0000013" ontologyURI="TestOntologyWebSite" />
  <ontologyTerm id="term11" term="ODE" sourceTermId="TestId:0000014" ontologyURI="TestOntologyWebSite" />
</ontologyTerms>
<model id="model1" name="Edelstein1996_EPSP_AChEvent" sourceURI="file://localFile" />
- <operations>
  - <operation id="op1" ontologyTerm="term2">
    <algorithm id="algo1" ontologyTerm="term1" />
    <software id="soft1" name="COPASI" version="COPASI 4.4 Build 26" uri="http://www.copasi.org" />
  - <result>
    + <resultComponent id="component11">
    + <resultComponent id="component2">
    + <resultComponent id="compenen31">
  </result>
```

Copasi Web

A Web User Interface to Copasi Web Services

[Home](#)
[Services Home](#)
[COPASI Home](#)

Available Services

Model Processor
[SBMLToCopasiML](#)
[CopasiMLToSBML](#)
[ValidateModel](#)

Steady State
 Synchronous
 Model
[CopasiML](#)
[SBML](#)

Asynchronous
 Model
[CopasiML](#)
[SBML](#)

```
<?xml version="1.0" encoding="UTF-8" ?>
- <sbrml xmlns="http://www.sbml.org/sbml/level1" version="1.0" level="1.0">
+ <ontologyTerms>
  <model id="model1" name="Edelstein1996_EPSP_AChEvent" sourceURI="file://localFile" />
- <operations>
  - <operation id="op1" ontologyTerm="term2">
    <algorithm id="algo1" ontologyTerm="term1" />
    <software id="soft1" name="COPASI" version="COPASI 4.4 Build 26" uri="http://www.copasi.org" />
  - <result>
    + <resultComponent id="component11">
      - <resultComponent id="component2">
        - <dimensionDescription>
          - <compositeDescription name="Reaction" ontologyTerm="term6" indexType="string">
            - <tupleDescription>
              <atomicDescription name="Flux" ontologyTerm="term7" valueType="double" />
              <atomicDescription name="Particle Flux" ontologyTerm="term8" valueType="double" />
            </tupleDescription>
          </compositeDescription>
        </dimensionDescription>
      - <dimension>
        - <compositeValue indexValue="React0">
          - <tuple>
            <atomicValue>4.98173e-18</atomicValue>
            <atomicValue>3.00007e+06</atomicValue>
          </tuple>
        </compositeValue>
      </dimension>
    </resultComponent>
  </result>
</operations>
</ontologyTerms>
</sbrml>
```



A Web User Interface to Copasi Web Services

- SBML
- Asynchronous Model
- CopasiML
- SBML
- Time Course
- Synchronous Model
- CopasiML
- SBML
- Asynchronous Model
- CopasiML
- SBML
- Parameter Estimation
- Asynchronous Model
- CopasiML
- SBML

```
<software id="soft1" name="COPASI" version="COPASI 4.4 Build 26" uri="http://www.copasi.org" />
- <result id="result1">
- <resultComponent id="component1">
- <dimensionDescription>
- <compositeDescription name="Time" ontologyTerm="term3" indexType="double">
- <compositeDescription name="Species" ontologyTerm="term4" indexType="string">
- <tupleDescription>
  <atomicDescription name="Concentration" ontologyTerm="term5" valueType="double" />
  <atomicDescription name="Particle Numbers" ontologyTerm="term6" valueType="Integer" />
</tupleDescription>
</compositeDescription>
</compositeDescription>
</dimensionDescription>
- <dimension>
- <compositeValue indexValue="0">
- <compositeValue indexValue="BasalACh2">
- <tuple>
  <atomicValue>0</atomicValue>
  <atomicValue>0</atomicValue>
</tuple>
</compositeValue>
+ <compositeValue indexValue="IntermediateACh">
+ <compositeValue indexValue="ActiveACh">
- <compositeValue indexValue="Active">
- <tuple>
  <atomicValue>0</atomicValue>
```

Conclusions

- SBRML provides a simple but powerful structure for representing simulation and experimental results
- Easy storage, retrieval, and exchange of simulation and experimental results
- Simplifies the reading of data in the context of biochemical model by software programs

Future Plans

- Feedback is solicited from the community!
- After feedback:
 - Adjustment of the Object Model and Schema
 - Further prototyping and demonstration
 - Development of library
 - libSBRML with API for C, C++, Java etc.

Link to documents: <http://www.comp-sys-bio.org>

Acknowledgements

We are grateful to the BBSRC and EPSRC for funding of this work through the Manchester Centre for Integrative Systems Biology.

Thanks!

Questions?