SBRML Interoperability

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THE MEETING

SBRML: Pedro Mendes, Joseph O. Dada
SED-ML: Nicolas Le Novére, Dagmar Waltemath, Frank T. Bergmann
Organizer: Sven Sahle
SYSTEMS BIOLOGY RESULTS
MARKUP LANGUAGE (SBRML)
SBRML - Overview

Joseph O. Dada et. al (2009)
SBRML - Operation

[Diagram of SBRML Operation with overlapping elements highlighted]

Joseph O. Dada et. al (2009)
SBRML - Results

Joseph O. Dada et. al (2009)
SBRML – Proposed Change I

• Move the result component (and downstream elements in the UML diagram) into its own namespace, as this is the primary component that would be referenced by SED-ML descriptions

• This would effectively separate the numerical components in SBRML from the descriptive components

• SBRML remains untouched otherwise, existing software that uses it can be quickly updated
The dimension description in SBRML refers to the one model that gave rise to the data.

By introducing a new indexType ‘xpath’ we will be able to reuse this indexing for the model referenced by SED-ML.
HOW DOES SBRML BENEFIT FROM SED-ML
SBRML references SED-ML

- The minimal change for SBRML is to add an optional attribute ‘source’ to the Method Element, which would allow it to reference the SED-ML simulation description (Or other formats).
- Other possible changes discussed include sub-classing the SBRML Model / Method or Operation class to add support for SED-ML elements there.
HOW AND TO GET IT INTO SED-ML
Use Cases

The newly extracted numerical core (dubbed NUML = NUmerical Markup Language) will be of interest in many places:

– Referencing previous Simulation Result to parameterize simulation.
– Reference external data in post processing (i.e. DataGenerators)
– Referencing (external) data in model pre-processing (i.e.: Model changes)
Externalize stuff

This could actually be in an external file.

Vital For SED-ML
Basic Idea

• Declare a way to index the data wherever it may come from

• Reference it in ChangeMath / DataGenerator and possible future simulation classes
Add ListOf<Data> to SED-ML

<listOfData>
  <dataFromSimulation id="data1" task="task1">
    <numl:dimensionDescription>
      <numl:compositeDescription numl:indexType="double">
        <numl:compositeDescription numl:indexType="xpath">
          <numl:atomicDescription numl:valueType="double"/>
        </numl:compositeDescription>
      </numl:compositeDescription>
    </numl:dimensionDescription>
  </dataFromSimulation>
</listOfData>
Add ListOf<Data> to SED-ML

```xml
<listOfData>
  <dataFromSimulation id="data1" task="task1">
    <numl:dimensionDescription>
      <numl:compositeDescription numl:indexType="double">
        <numl:compositeDescription numl:indexType="xpath">
          <numl:atomicDescription numl:valueType="double"/>
        </numl:compositeDescription>
      </numl:compositeDescription>
    </numl:dimensionDescription>
  </dataFromSimulation>
</listOfData>
```

Similarly for other data: “externalData” would just have a source attribute instead of a task. “data” could inline data using “numl:dimension”
Using the ListOf<Data>

• After the values are declared, their identifiers could be used in all MathML expressions!

• SED-ML L1V1 already introduces the MathML Lambda element!

• This would allow us to use the aforementioned definitions as:

  – value = data1(time, variable)
Thoughts / Questions?

• Get involved:
  – sed-ml-discuss@lists.sourceforge.net

• More information:
  – http://sed-ml.org/
  – http://sbrml.sourceforge.net/