CORE SBML MODELS

Biological Content:
- Reactions
- Species
- Parameters
- Compartments
- Functions
- Events
- Math
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- Reactions
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- Math
Hierarchical Model Composition Models ('COMP')

- Biological Content:
  - Reactions
  - Species
  - Parameters
  - Compartments
  - Functions
  - Events
  - Math
THREE BASIC TASKS:

- Define multiple models
- Import copies as submodels
- Connect their elements
1 DEFINE MULTIPLE MODELS

Model

Document
2 Import copies as submodels

Model

Reactions
Species
Compartments etc.

Submodels

Model Definition
Model Definition
Model Definition
External Model Definition
Model Definition
External Model Definition

Document

2 IMPORT COPIES AS SUBMODELS

- Model Definition
- Model Definition
- Model Definition
- External Model Definition
- Model Definition
- External Model Definition

Reactions
Species
Compartments etc.

Model

Submodels
submod1
2 Import copies as submodels

Model
Reactions
Species
Compartments
etc.

Submodels
submod1
submod2
submod3
2 IMPORT COPIES AS SUBMODELS

Model Definition

Model Definition

Model Definition

External Model Definition

Model Definition

External Model Definition

Reactions
Species
Compartments etc.

Model

Submodels

submod1

submod2

submod3

submod4

submod5
2 IMPORT COPIES AS SUBMODELS

Model Definition

Reactions
Species
Compartments etc.

Model Definition

External Model Definition

Model

External Model Definition

Submodels

submod1

submod2

submod3

Document
2 IMPORT COPIES AS SUBMODELS

Model

Submodels

submod1: Reactions, Species, Compartments...

submod2: Species, Events

submod3: Reactions, Species, Events

Reactions
Species
Compartments etc.
3 CONNECT THEIR ELEMENTS
COMPLICATION 1: DELETIONS

- $A \rightarrow B; k_0 A$
- $C \rightarrow B; k_0 C$
- $B \rightarrow ; k_0 B$
- $B + C \rightarrow D; k_0 C B$
- $X \rightarrow Y; k_0 B$
- $\frac{dB}{dt} = -2.2$

Compliation 1: Deletions

\[ A \rightarrow B \quad \text{k0*A} \]
\[ B \rightarrow \quad \text{k0*B} \]
\[ B + C \rightarrow D \quad \text{k0*C*B} \]
\[ C \rightarrow B \quad \text{k0*C} \]
\[ X \rightarrow Y \quad \text{k0*B} \]
\[ dB/dt = -2.2 \]
COMPLICATION 1: DELETIONS

A → B; k₀*A
C → B; k₀*C
B → ; k₀*B
C → B; k₀*C
B + C → D; k₀*C*B

X → Y; k₀*B
dB/dt = -2.2

COMPLICATION 2: CONVERSION FACTORS

A → B; $k_0 \times A$

B → ; $k_0 \times B$

C → B; $k_0 \times C$

$B + C \rightarrow D; k_0 \times C \times B$

millimolar

molar
COMPLICATION 2: CONVERSION FACTORS

A → B; k0*A

C → B; k0*C

B → ; k0*B

C → B; k0*C

B + C → D; k0*C*B

cf: .001

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COMPLICATION 3: PORTS

Reactions
Species
Compartments etc.

Model

Submodels

submod1
B, C

submod2
A, B

submod3
A, B

submod4
B, D, F

submod5
D, E

PART II: XML STRUCTURES
Submodel

id: SId
modelRef: SIdRef
lengthConversionFactor: SIdRef {use="optional"}
areaConversionFactor: SIdRef {use="optional"}
volumeConversionFactor: SIdRef {use="optional"}
substanceConversionFactor: SIdRef {use="optional"}
timeConversionFactor: SIdRef {use="optional"}
extentConversionFactor: SIdRef {use="optional"}

listOfDeletions
0,1

ListOfDeletions
deletion
0,...,*

Deletion
id: SId {use="optional"}
**SBaseRef**

- port: PortSIdRef {use="optional"}
- idRef: SIdRef {use="optional"}
- unitRef: UnitSIdRef {use="optional"}
- metaIdRef: IDREF {use="optional"}

sbaseRef

0,1
POTENTIAL ISSUE:
CONVERSION FACTORS
<table>
<thead>
<tr>
<th>Component</th>
<th>Attribute value</th>
<th>Automatic conversion factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>AlgebraicRule</td>
<td>(All)</td>
<td>1</td>
</tr>
<tr>
<td>AssignmentRule</td>
<td>(All)</td>
<td></td>
</tr>
<tr>
<td>Compartment</td>
<td>spatialDimensions=&quot;1&quot;</td>
<td>lengthConversionFactor</td>
</tr>
<tr>
<td>Compartment</td>
<td>spatialDimensions=&quot;2&quot;</td>
<td>areaConversionFactor</td>
</tr>
<tr>
<td>Compartment</td>
<td>spatialDimensions=&quot;3&quot;</td>
<td>volumeConversionFactor</td>
</tr>
<tr>
<td>Compartment</td>
<td>spatialDimensions not equal to “1”, “2”, or “3”</td>
<td>1</td>
</tr>
<tr>
<td>Constraint</td>
<td>(All)</td>
<td>(None needed)</td>
</tr>
<tr>
<td>Delay</td>
<td>(All)</td>
<td>timeConversionFactor</td>
</tr>
<tr>
<td>EventAssignment</td>
<td>(All)</td>
<td>Conversion factor for referenced object</td>
</tr>
<tr>
<td>FunctionDefinition</td>
<td>(All)</td>
<td>1</td>
</tr>
<tr>
<td>InitialAssignment</td>
<td>(All)</td>
<td>Conversion factor for referenced object</td>
</tr>
<tr>
<td>KineticLaw</td>
<td>(All)</td>
<td>extentConversionFactor</td>
</tr>
<tr>
<td></td>
<td>implied rate of change of a species</td>
<td>timeConversionFactor</td>
</tr>
<tr>
<td>Parameter</td>
<td>(All)</td>
<td>1</td>
</tr>
<tr>
<td>Priority</td>
<td>(All)</td>
<td>1</td>
</tr>
<tr>
<td>RateRule</td>
<td>(All)</td>
<td>Conversion factor for referenced object</td>
</tr>
<tr>
<td></td>
<td></td>
<td>timeConversionFactor</td>
</tr>
<tr>
<td>Species</td>
<td>hasOnlySubstanceUnits=&quot;true&quot;</td>
<td>substanceConversionFactor</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Species</td>
<td>hasOnlySubstanceUnits=&quot;false&quot;</td>
<td>substanceConversionFactor</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Species</td>
<td>hasOnlySubstanceUnits=&quot;true&quot; replaced by a Species having hasOnlySubstanceUnits=&quot;false&quot;</td>
<td>substanceConversionFactor</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Compartment size</td>
</tr>
<tr>
<td>Species</td>
<td>hasOnlySubstanceUnits=&quot;false&quot; replaced by a Species having hasOnlySubstanceUnits=&quot;true&quot;</td>
<td>substanceConversionFactor</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Compartment size)</td>
</tr>
<tr>
<td>SpeciesReference</td>
<td>(All)</td>
<td>1</td>
</tr>
<tr>
<td>Trigger</td>
<td>(All)</td>
<td>(None needed)</td>
</tr>
<tr>
<td>(Unknown)</td>
<td>(All)</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 3: Conversion factors used for the different components defined by SBML Level 3 Core.
POTENTIAL ISSUE: CONVERSION FACTORS

- Perhaps remove conversion factors for submodels?
- Retain conversion factors for replacements
- Parameters unconverted anyway...
PART III: EXISTING IMPLEMENTATIONS
LIBSBML-COMP

- All classes implemented
- Get/set all attributes
- Add/remove all children
- Requires libSBML 5.1.0
- libsbml/5.1-packages-beta/comp-5.1.0-beta-1.zip

In-progress: convenience functions
  - Flattening
  - Submodel instantiation
Read/write hierarchical models!

In-progress:
- Replace rules more robustly
- Introduce deletions

Can only ‘replace’ elements with ids.
...and members of sbml-discuss and sbml-comp