

SBML multistate/multicomponent species mini-workshop 2007: Basic goals

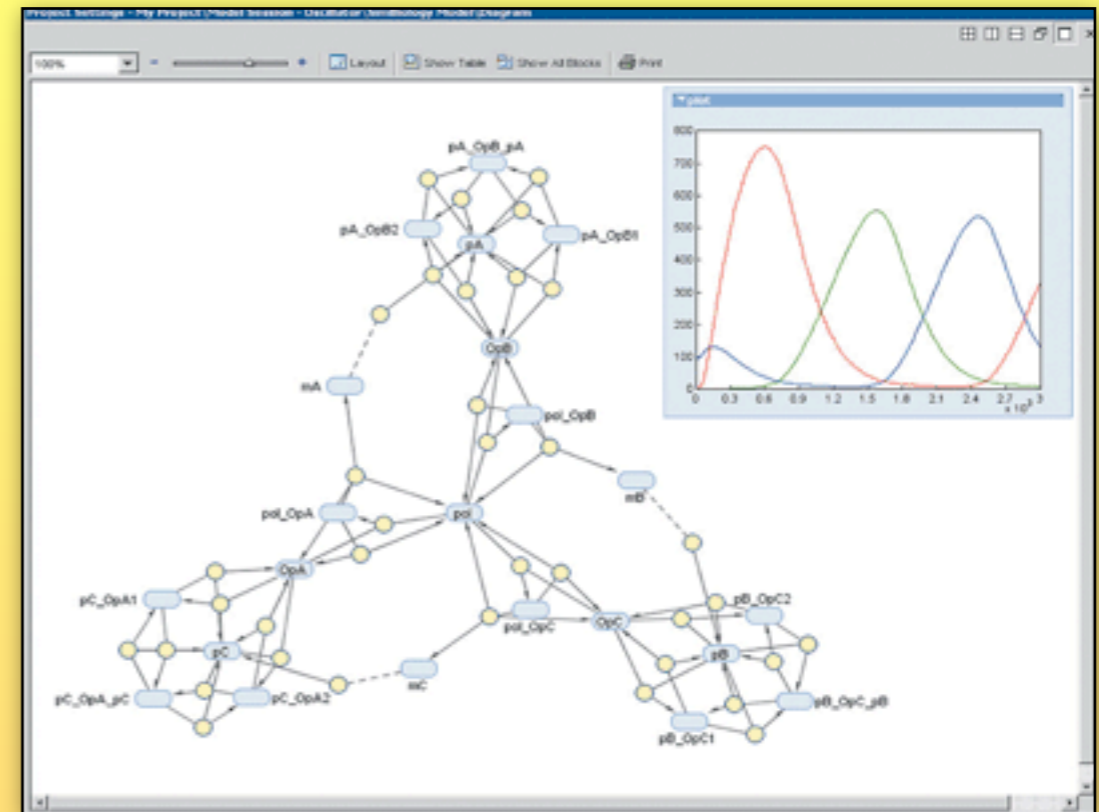
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Application's internal object model \neq SBML

```
<listOfSpecies>
  <species compartment="cytosol" id="ES" initialConcentration="1" />
  <species compartment="cytosol" id="P" initialConcentration="1" />
  <species compartment="cytosol" id="S" initialConcentration="1" />
  <species compartment="cytosol" id="E" initialConcentration="1" />
</listOfSpecies>
<listOfReactions>
  <reaction id="veg">
    <listOfReactants>
      <speciesReference species="E"/>
      <speciesReference species="S"/>
    </listOfReactants>
    <listOfProducts>
      <speciesReference species="ES"/>
    </listOfProducts>
    <kineticLaw>
      <math xmlns="http://www.w3.org/1998/MathML">
        <apply>
          <times/>
          <ci>cytosol</ci>
          <apply>
            <minus/>
            <apply>
              <times/>
              <ci>kon</ci>
              <ci>E</ci>
              <ci>S</ci>
            </apply>
            <apply>
              <times/>
              <ci>koff</ci>
              <ci>ES</ci>
            </apply>
          </apply>
        </math>
      </kineticLaw>
    </reaction>
  </listOfReactions>
```

SBML file

Application translates into internal data format



Application

- ◎ SBML is an object model + protocols for its use
- ◎ XML is a serialization of that object model

Modularizing SBML

◎ The future of SBML

- Major extensions have been requested and are sorely needed
- But SBML is complicated enough
 - Only the largest-scale efforts have implemented most of Level 2

◎ Idea (a natural one): modularize

- Layer additional language extensions on top of a core
 - Similar to XML: XML is core, then there's XPath, MathML, etc.
- Additional benefits:
 - Can decouple development of individual extensions
 - Software can recognize & work with extensions it needs

Candidate mechanism: XML namespaces

```
<sbml xmlns="http://www.sbml.org/sbml/level3/version1"  
      xmlns:multi="http://www.sbml.org/extensions/multi/version1">  
  <model id="example">  
    <listOfSpeciesTypes>  
      <speciesType id="A">  
        <multi:listOfStateVariables>  
          <multi:stateVariable id="x1" />  
        </multi:listOfStateVariables>  
      </speciesType>  
      ...  
    ...  
  </model>  
</sbml>
```

What will be the core?

- ⊙ Expected to be *mostly* Level 2 Version 3, but ...
- ⊙ Chicken-and-egg problem: don't know if will need crucial features in the core to support extensions until we know what the extensions are
- ⊙ Current plan:
 1. Develop draft proposals for major extensions on the table
 2. Examine them together
 3. *Then* decide what needs to go into SBML Level 3 Core

What are expected Level 3 extensions?

| Extension | Code name |
|-------------------------------|-----------|
| Arrays | L3A |
| Composition | L3C |
| Distributions & ranges | L3D |
| Diagram layout | L3L |
| Diagram rendering | L3R |
| Multistate/multicomp. species | L3M |
| Spatial geometry | L3S |
| Dynamic structures | L3Y |

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◎ Extra credit: extension to libSBML to support reading/writing format