

Why inserting modularity in the core  
package of Level 3

(implementing *aggregation* in the core)

# Why?

- Breaking the rule 1 SBML=1 model=1 file
- Monolithic models are unmaintainable (thousands of species)
- Using a given element (e.g. species) with different units in different context
- Paving the way to model composition etc.
- Improving interoperability with CellML

# How?

- Build on CellML experience (see sec 3.3 ex 4), with SBML thoroughness ...
  - Encapsulate ALL elements into modules.  
“model” is a module
  - A module can contain any number of any element (even 0)
  - A module may expose variables as port
  - A module contains its own set of namespaces
  - A variable output of a module can be mapped to a variable input to another module.

- Andrew's xlink target modules' ports
- Unit conversion takes place between output and input variable => e.g. species unit conversion not anymore implicitly in the “stoichiometry”

```
file xxxxx
<SBML>
import file yyyyy
import file zzzzzz
```

```
<model>
mapping
```

```
A.x <=> B.y
```

```
file yyyyy
```

```
module A
```

```
species X unit="mole"
           status="port"
           direction="out"
```

```
species Y
parameter k
```

```
reaction foo
```

```
Y => X ; X=k.Y
```

```
module B
```

```
species M unit="micromole"
           status="port"
           direction="out"
```

```
species N
parameter k
```

```
reaction bar
```

```
M => N ; N=k.M
```

## Reduced version : Only 1 file

```
file xxxxx  
<SBML>
```

```
<model>  
mapping
```

```
A.x <=> B.y
```

```
module A
```

```
species X unit="mole"  
          status="port"  
          direction="out"
```

```
species Y  
parameter k
```

```
reaction foo
```

```
Y => X ; X=k.Y
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```
module B
```

```
species M unit="micromole"  
          status="port"  
          direction="out"
```

```
species N  
parameter k
```

```
reaction bar
```

```
M => N ; N=k.M
```

# MyModel.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml name="MyModel" xmlns="http://www.sbml.org/sbml/level3">
  <listOfImports>
    <!-- I DECLARE THAT IN ADDITION OF THIS FILE,
          SOME MODULES ARE FOUND IN OTHER FILES-->
    <!-- THE ORDER OF THE IMPORT IS IMPORTANT -->
    <import file="charybde.xml" />
    <import file="scylla.xml" />
  </listOfImports>
  <model>
    <listOfModules>
    <!-- THIS MODEL REQUIRES THE MODULE A AND B -->
    <!-- THE ORDER OF DECLARATION IS IMPORTANT-->
    <module name="A" />
    <module name="B" />
    </listOfModules>
    <listOfMappings>
    <mapping var1="A.MEKPP" var2="B.MAPKKPP" />
    </listOfMappings>
    <listOfCompartments>
    <!-- THIS COMPARTMENT WILL BE KNOWN BY EVERYONE -->
    <compartment id="cell" size="1"/>
    </listOfCompartments>
  </model>
</sbml>
```

# charybde.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml name="MyModel" xmlns="http://www.sbml.org/sbml/level3">
  <module id="B">
    <listOfUnitDefinitions>
      <!-- DEFAULT SUBSTANCE UNIT IS REDEFINED TO MICROMOLE -->
      <unitDefinition id="substance" name="micromole">
        <listOfUnits>
          <unit kind="mole" scale="-6" />
        </listOfUnits>
      </unitDefinition>
    </listOfUnitDefinitions>
    <listOfSpecies>
      <!-- THIS INITIALCONCENTRATION OVERRIDE THE ONE DECLARED IN MODULE A -->
      <species id="MAPKKPP" compartment="cell" initialConcentration="0" status="port" direction="in" />
      <species id="MAPK" compartment="cell" initialConcentration="1" />
      <species id="MAPKPP" compartment="cell" initialConcentration="0" />
    </listOfSpecies>
    <listOfParameters>
      <parameter id="kcat" />
      <parameter id="Km" />
    </listOfParameters>
    <listOfReactions>
      <listOfReactants>
        <speciesReference species="MAPK" />
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="MAPKPP" />
      </listOfProducts>
      <listOfModifiers>
        <speciesReference species="MAKKPP" />
      </listOfModifiers>
      <kineticLaw>
<!--          ... kcat * MAKKPP * MAPK / (Km + MAPK) * cell          -->
      </kineticLaw>
    </listOfReactions>
  </module>
  <module id="C" /> <!-- something we do not care about -->
</sbml>
```



# scylla.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<sbml name="MyModel" xmlns="http://www.sbml.org/sbml/level3">
  <module id="A">
    <listOfSpecies>
      <!-- NOTE THAT UNITS ARE NOT DEFINED => BUILT-IN -->
      <species id="MEK" compartment="cell" initialConcentration="1e-5"/>
      <species id="MEKPP" compartment="cell" initialConcentration="1e-5" status="port" />
    </listOfSpecies>
    <listOfParameters>
      <parameter id="Vmax" />
      <parameter id="Km" />
    </listOfParameters>
    <listOfReactions>
      <listOfReactants>
        <speciesReference species="MEK"/>
      </listOfReactants>
      <listOfProducts>
        <speciesReference species="MEKPP" />
      </listOfProducts>
      <kineticLaw>
<!--      ... Vmax * MEK / (Km + MEK) * cell      -->
      </kineticLaw>
    </listOfReactions>
  </module>
</sbml>
```