SBML and FBA models revisited

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Previous work: Karthik Raman 2005

Critical points

- FBA is an *operation* performed on a model, essentially specified by the objective function, unlike a kinetic model *definition*
  - Flux bounds may be biochemical constraints on the model (or based on the simulation)
- ***Fundamental question***: should SBML also allow
  - exchange of simulation results (flux values), esp. for FBA?
  - Specification of a model *instance*, in terms of a particular objective function

The itch: why I'm interested in this

- Currently working on applying constraint based modelling to ecosystems using existing genome scale models
- Many model descriptions exist in a variety of formats:
  - Excel spreadsheets (smaller models)
  - Text files (Simpheny)
  - COBRA generated sbml (BiGG database)
- There is growing interest in using constraint based model descriptions further analysis

Karthik called this a workaround: COBRA sbml

```
</reaction>
<reaction id="R_EX_his_L_LPAREN_e_RPAREN_" name="L-Histidine exchange" reversible="true
<notes>
<html:p>Abbreviation: R_EX_his_L_LPAREN_e_RPAREN_</html:p>
<html:p>Synonyms: _0</html:p>
<html:p>Equation: [e] : his-L &lt;==&gt;</html:p>
<html:p>Confidence Level: </html:p>
</notes>
<listOfReactants>
<speciesReference species="M_his_DASH_L_e" stoichiometry="1"/>
</listOfReactants>
<listOfProducts>
<speciesReference species="M_his_DASH_L_b" stoichiometry="1"/>
</listOfProducts>
<kineticLaw>
<math xmlns="http://www.w3.org/1998/Math/MathML">
<ci>FLUX_VALUE</ci>
</math>
<listOfParameters>
<parameter id="LOWER_BOUND" value="0" units="mmol_per_gDW_per_hr"/>
<parameter id="UPPER_BOUND" value="999999" units="mmol_per_gDW_per_hr"/>
<parameter id="OBJECTIVE_COEFFICIENT" value="0" />
<parameter id="FLUX_VALUE" value="0" units="mmol_per_gDW_per_hr"/>
</listOfParameters>
</kineticLaw>
</reaction>
```

model output, units?

Workaround continued

```
<species id="M_his_DASH_L_c" name="L-Histidine_C6H9N3O2“
    compartment="Cytosol“  charge="0" boundaryCondition="false"/>

<species id="M_his_DASH_L_e" name="L-Histidine_C6H9N3O2"
    compartment="Extraorganism“  charge="0" boundaryCondition="false"/>

<species id="M_his_DASH_L_b" name="L-Histidine_C6H9N3O2“
    compartment="Extraorganism" charge="0" boundaryCondition="false"/>
```

Discussion

- A level 3 module for flux/constraint based models?
  - reaction bounds
  - objective function(s)
- Additional attributes (or annotations)?
  - reactions: exchange, subsystem, ec number
  - species: molecular composition
- FBA software
  - COBRA, BiGG, Simpheny
  - SBW
  - PySCeS (soon)
  - FluxAnalyzer, CellAnalyzer, Fluxor?
- Representing an FBA simulation experiment?