SBML and FBA models revisited

Brett G. Olivier

Dept. of Molecular Cell Physiology
Vrije Universiteit Amsterdam
Amsterdam, The Netherlands

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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 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?