Systems Biology Pathway Exchange (SBPAX)

Gluing SBML-type Models to BioPAX-type Pathways

Oliver Ruebenacker

Virtual Cell, Center for Cell Analysis and Modelling
BioPAX-OBO

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Outline

SBML and BioPAX

SBML

- "System Biological Markup Language"
- Kinetic Modelling
- XML
- reactions, species
- No term hierarchy

BioPAX

- "Biological Pathway Exchange"
- Qualitative, no kinetics
- RDF
- interactions, physical entities
- Hierarchy of Terms

The SBML-BioPAX Integration Challenge

Motivation: Both communities possess enormous amounts of public data on cellular reaction networks.

Challenge: Purposes have been diverging and therefore terms are incompatible.

Conversions and Annotations

Conversions

- e.g. Binom (Cytoscape), sbml2biopax (`sbml.org`)
- file $\Leftrightarrow$ file
- reaction $\Leftrightarrow$ conversion
- species $\Leftrightarrow$ physicalEntity

Annotation

- e.g. J Luciano and J Zucker
- Use BioPAX for annotations in SBML
- Add info about conversion or physical entity to species or reaction

How Far We Get With Conversions And Annotations

Pro: One-to-one map between SBML and BioPAX often considered useful

Contra: In general, one-to-one map is wrong

SBML-SBPAX-BioPAX Repository

Requirements

- Relationships between SBML and BioPAX terms.
- Terms compatible with both SBML and BioPAX
- Identify and reconcile semantic differences

SBML-SBPAX-BioPAX Joint RDF Repository

SBML

SBML data objects (RDF Reflection)

SBPAX

Relationships between SBML and BioPAX objects

BioPAX

BioPAX data objects

System Model

SBML

- File boundaries delineate models

BioPAX

- There is no model
- File boundaries not delineations

System Model (SBPAX)

- Introduce term system model
- System model links to its components
- Advantage: Easy to re-use objects for different models

Species and Physical Entities

Species (SBML)

- No ID restrictions
- Compartment hierarchy
- Species can be anything
- Species depend on model

Physical Entity (BioPAX)

- Hybrid ID specs
- ID by sequence for DNA, RNA, proteins
- ID by chemical structure for "small molecule"
- ID unclear for complexes
- No compartment hierarchy

Substance (SBPAX)

- Hierarchy of substance IDs: Sequence, chemical structure, organism, location

Reactions and Conversions

Reaction (SBML)

- Continuous flux from pool to pool
- Controls included

Conversion (BioPAX)

- Discrete event, discrete participants
- Controls separate objects

Reactions (SBPAX)

- Distinguish between individual reaction and reaction ensemble
- Substance hierarchy $\Rightarrow$ Reaction hierarchy
- Terms for controls

Reactions and Reaction Models

Reaction (SBML)

- Kinetic
- Approximate rate laws
- Modeller's choices

Conversion (BioPAX)

- No kinetics
- No approximations
- No choices

Reaction and Reaction Model (SBPAX)

- Need to distinguish between reaction and reaction model
- Reaction only objective truths, no approximations or modeller's choices
- Reaction Model includes kinetics, which are approximate and contain modeller's choices

Stoichiometry

SBML

- Stoichiometry merely rate law book keeping

BioPAX

- Actual numbers of participants

SBPAX

- Distinguish between real and effective stoichiometry
- Objective real numbers of participants
- Effective stoichiometry can be any multiple

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