SBOL Modeling Extension

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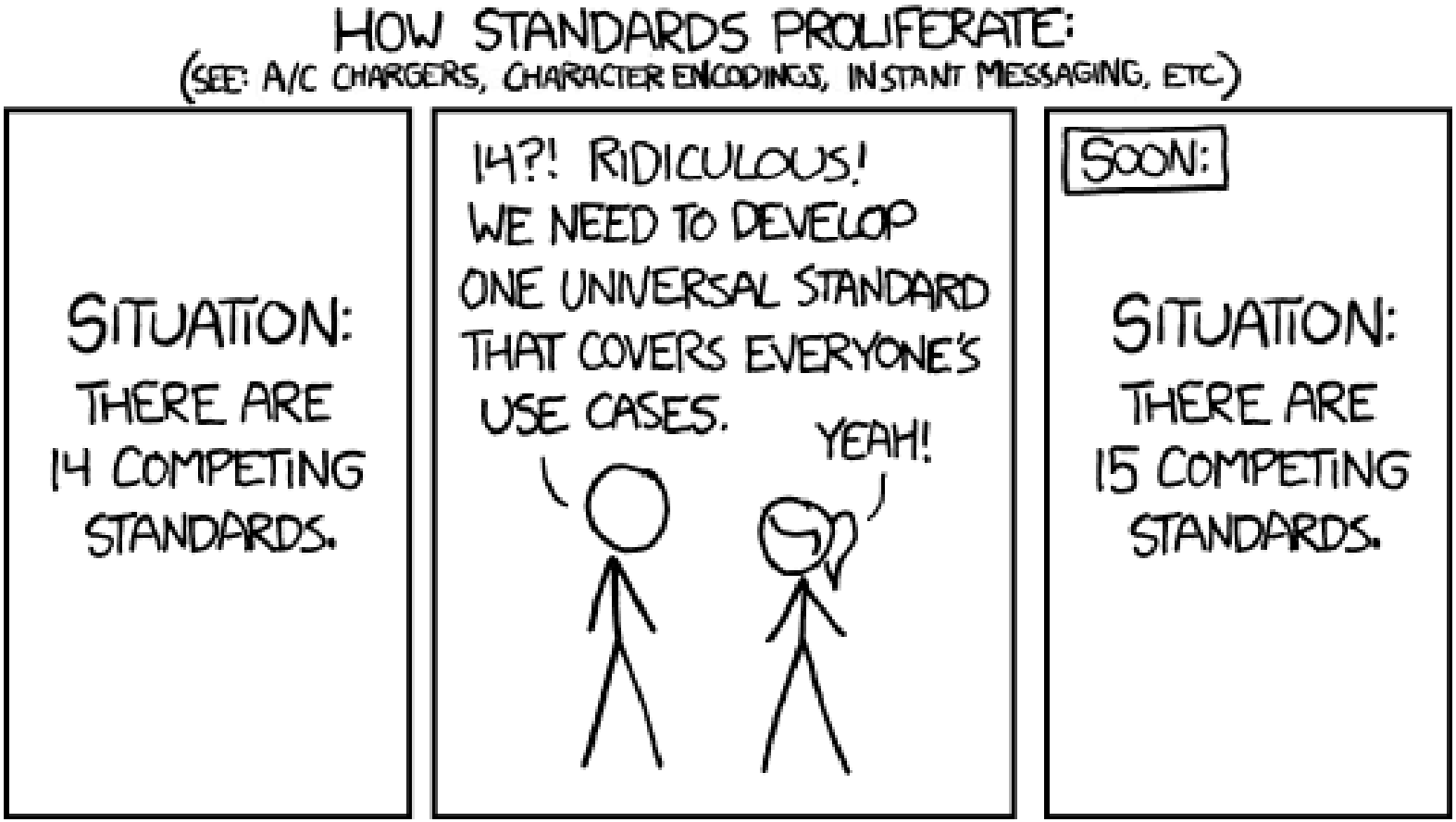
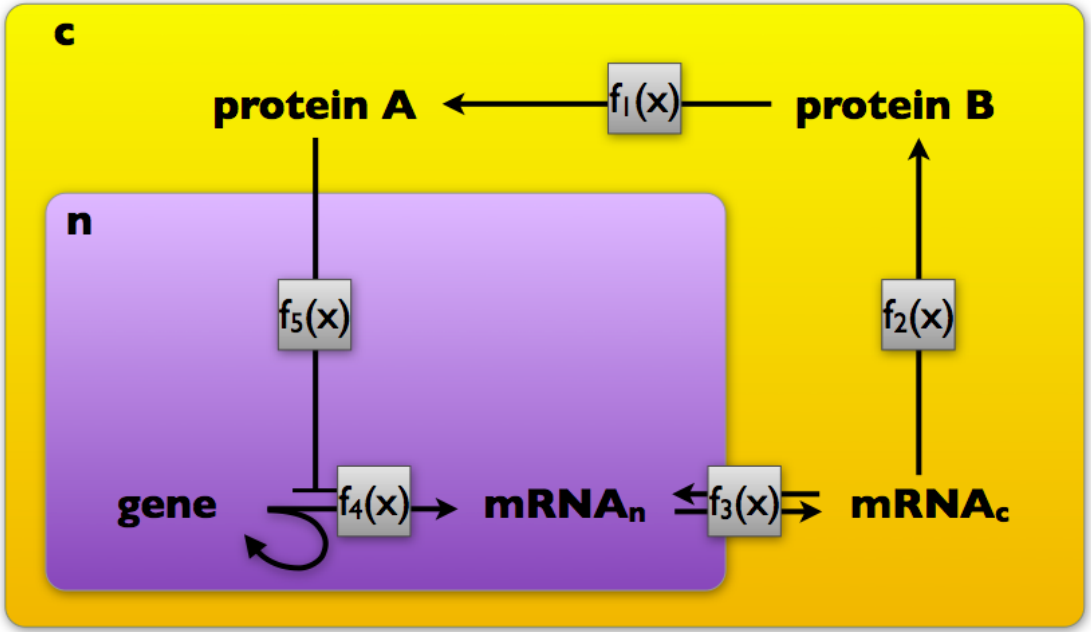
Motivation

- SBOL currently only includes structural information.
- Recently added device class provides location to link modeling extension.
- The SBOL modeling extension will add behavioral information.
- This information should be sufficient to enable:
  - *Synthesis* - selection of DNA components to perform a desired behavior.
  - *Analysis* - check through simulation or other means that a design provides a desired behavior.
- This extension requires:
  - Logical relationships (i.e., a gene product represses a promoter).
  - Quantitative information (i.e., the binding affinity of the repressor).

A Word of Warning

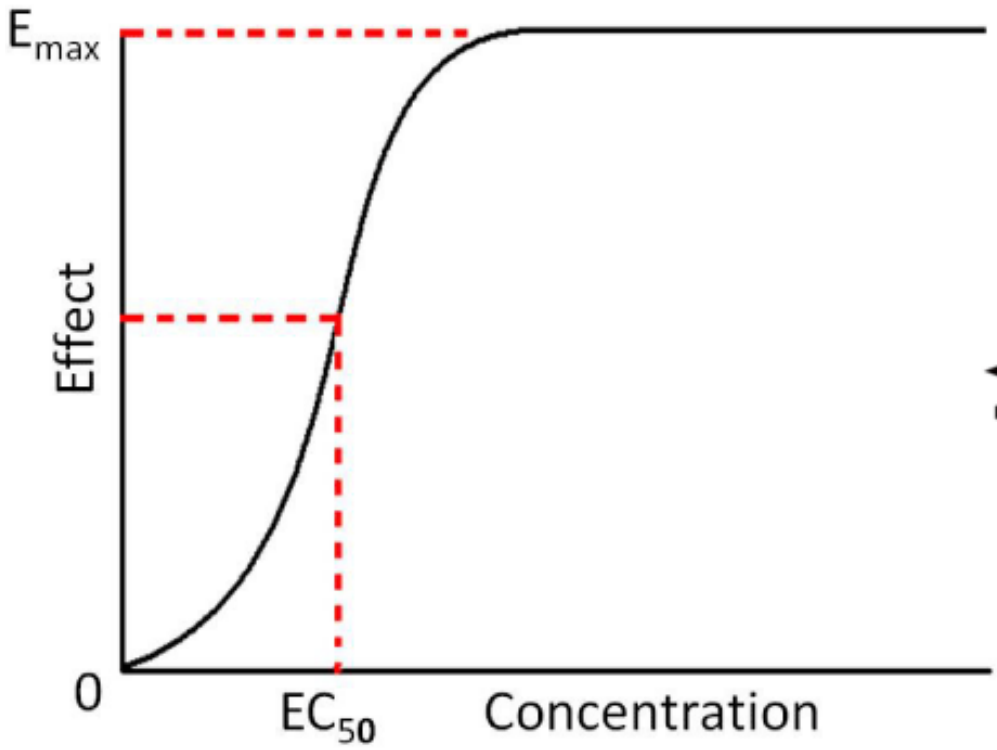


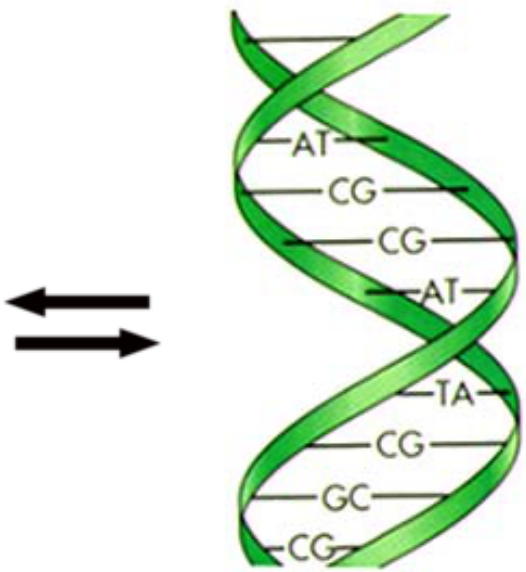
Systems Biology Modeling Language (SBML)



- Supported by >250 tools, enabling researchers to create, annotate, simulate, and visualize models, and archive in the BioModels database.
- SBML also has *parameters*, *functions*, *unit definitions*, *initial assignments*, *rules* for continuous relationships, *events* for discontinuous state changes, and *constraints* to indicate when a simulation should terminate.
- Numerous packages have been proposed including *layout*, *hierarchical model composition*, *spatial processes*, *flux balance constraints*, etc.

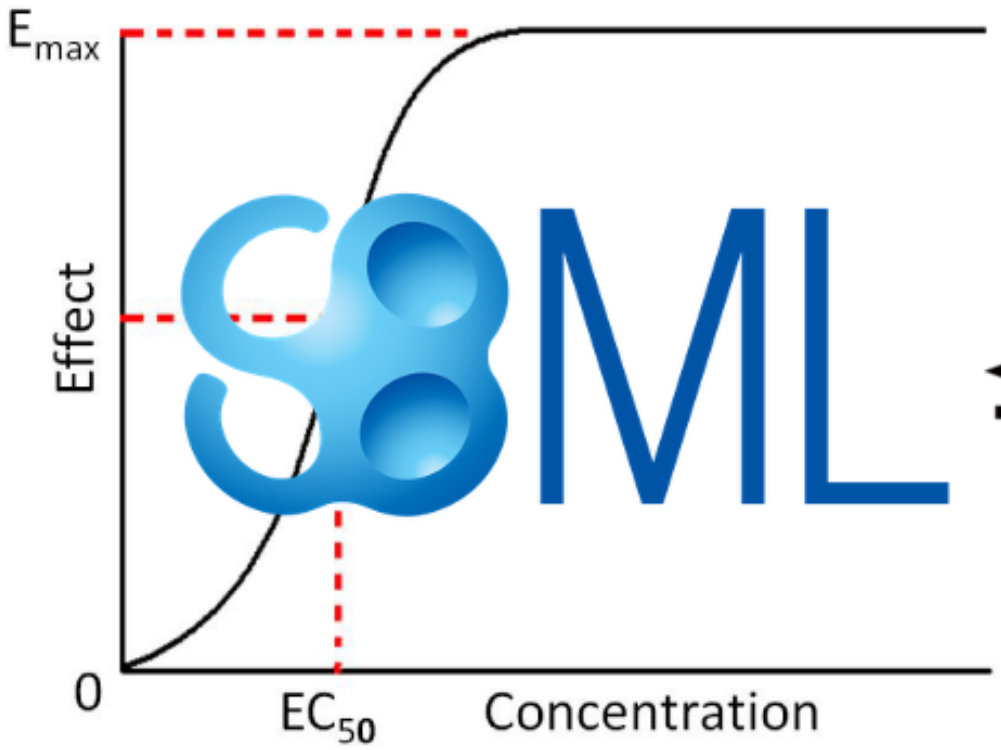
Coupling Models and DNA

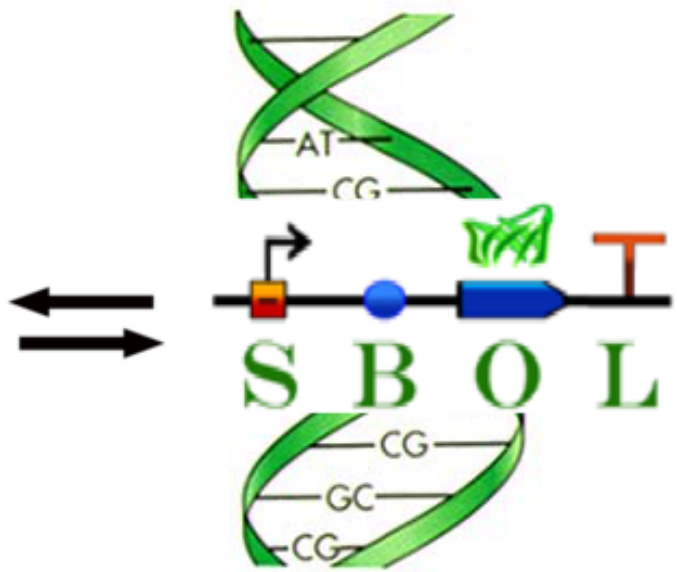




Model DNA Component

Coupling Models and DNA





Model DNA Component

RDF/XML SBML-to-SBOL Annotation

RDF/XML SBML-to-SBOL Annotation

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  <annotation>
    <ModelToSBOL xmlns="http://sbolstandard.org/modeltosbol/1.0#">
      <rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"
               xmlns:mts="http://sbolstandard.org/modeltosbol/1.0#">
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          <mts:DNAComponents>
            <rdf:Seq>
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</SBML_ELEMENT>
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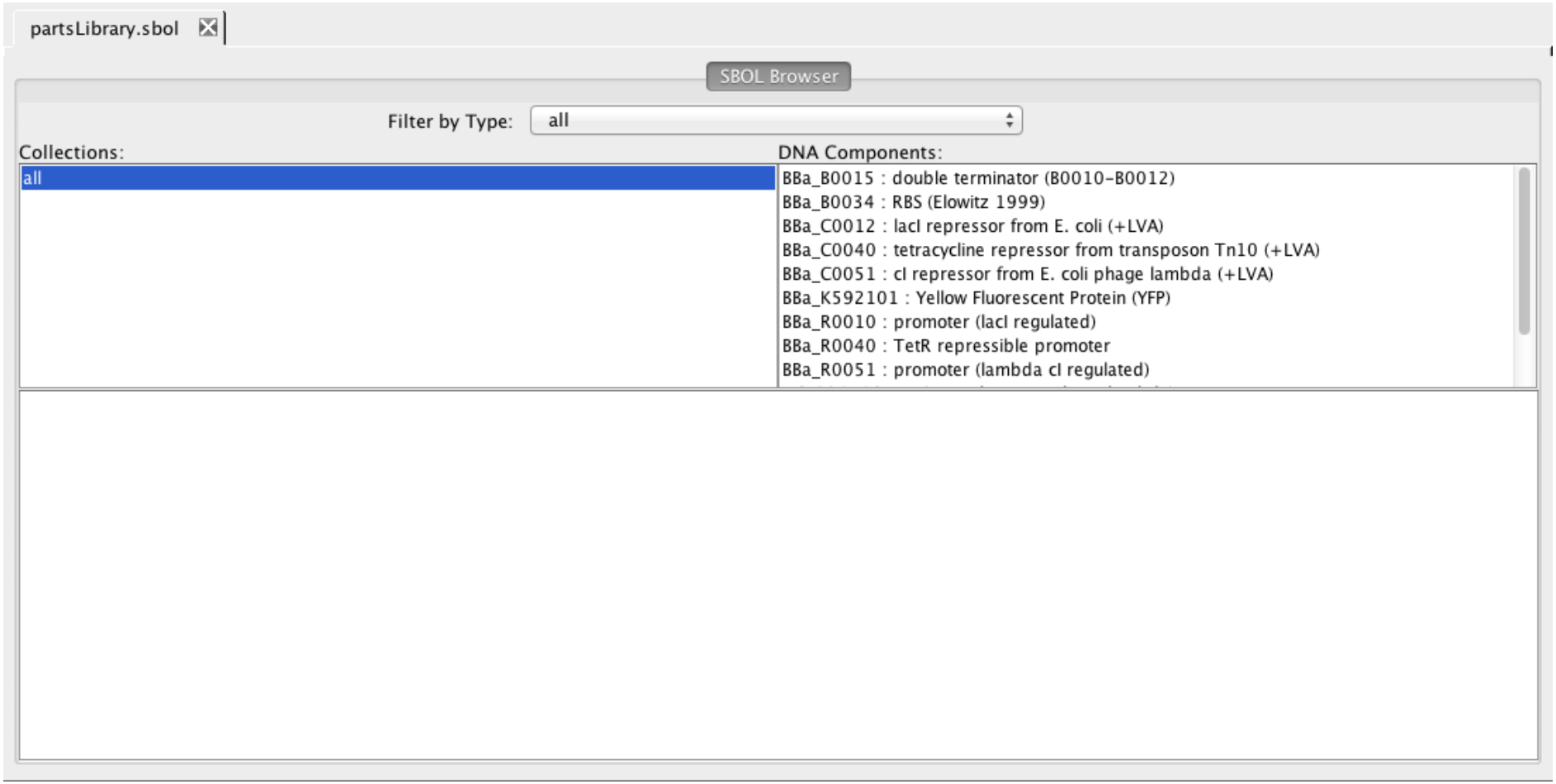
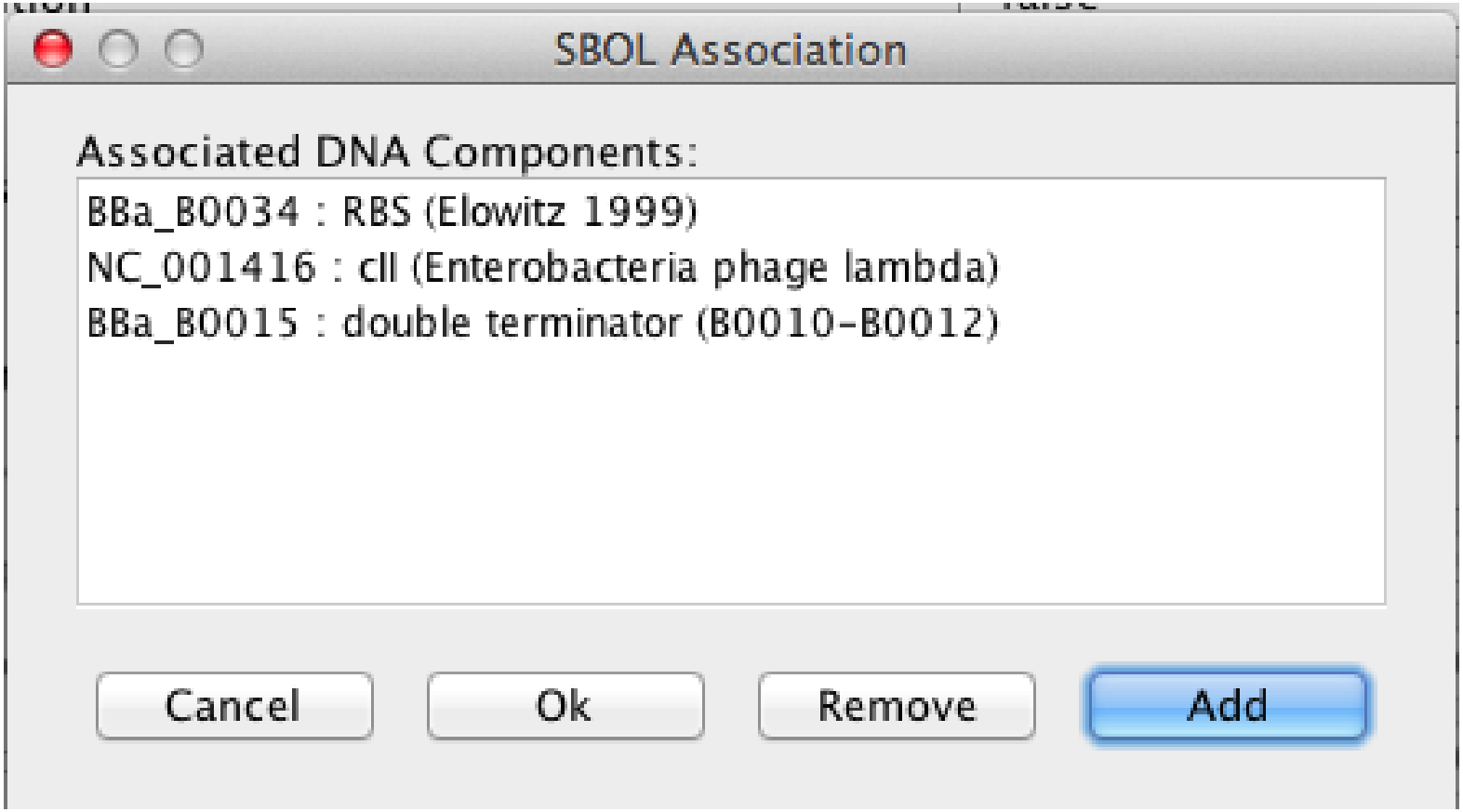
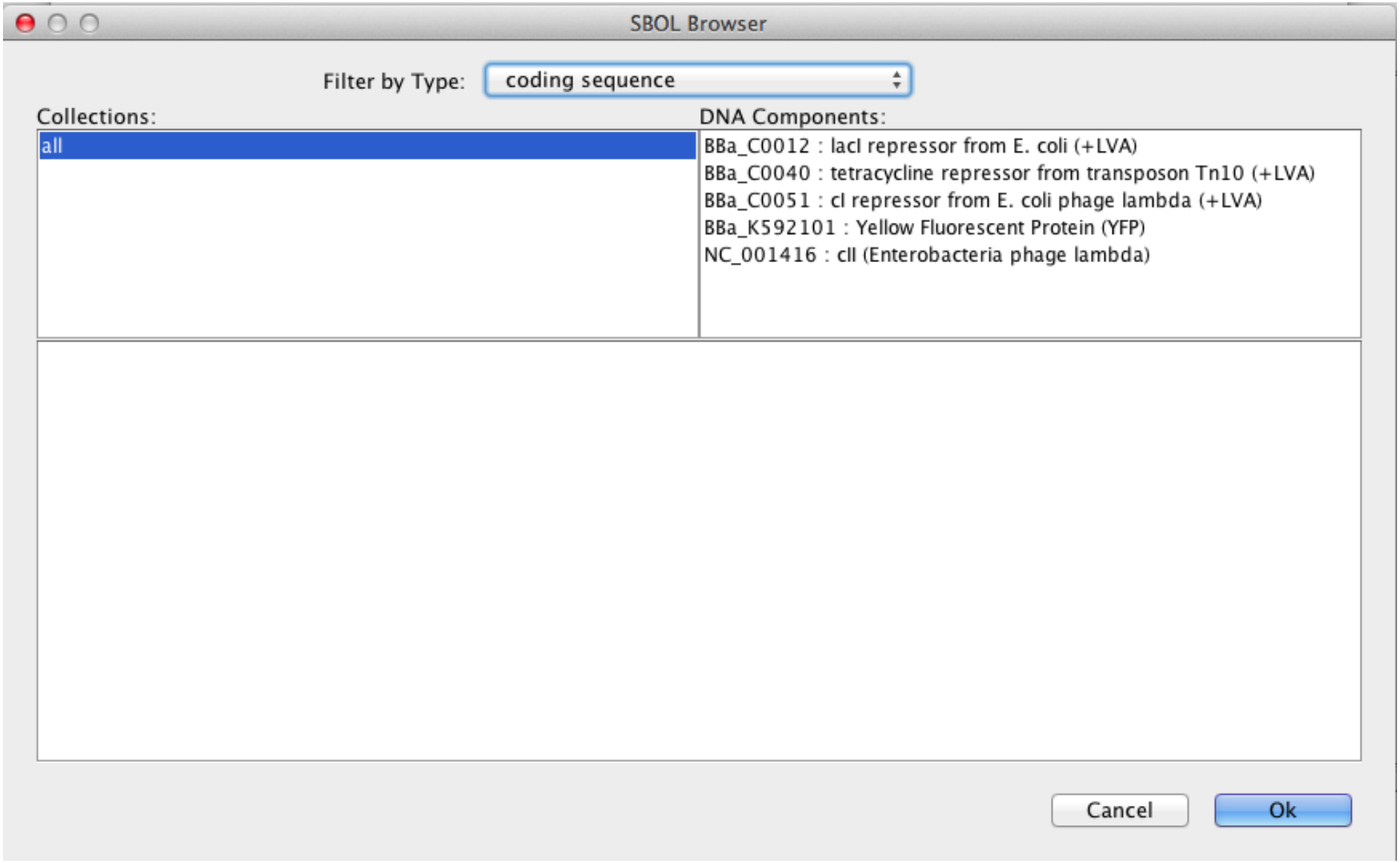
SBOL Browser



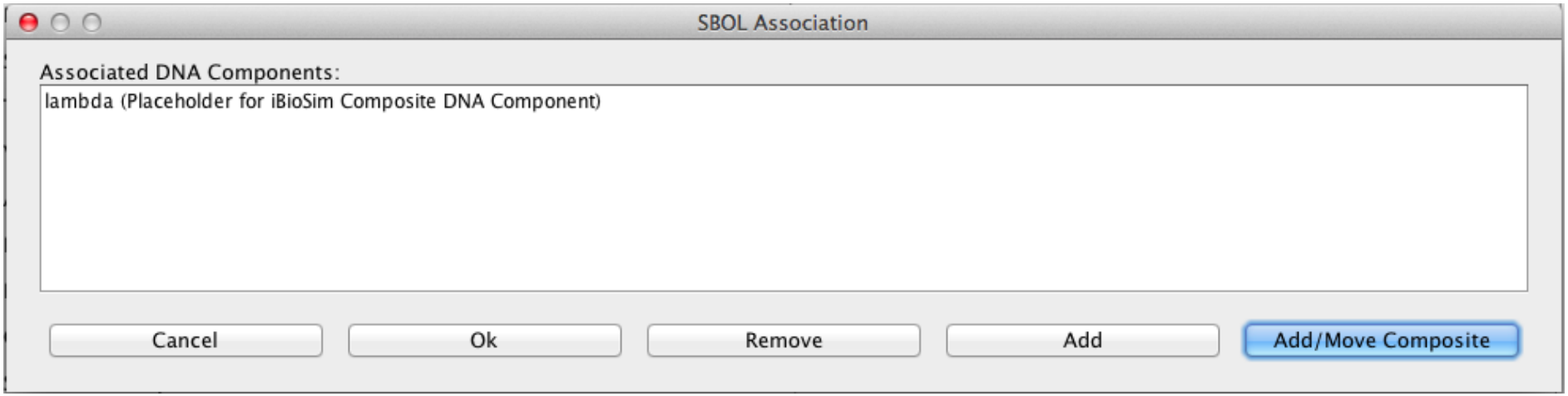
Associate SBOL to SBML Element



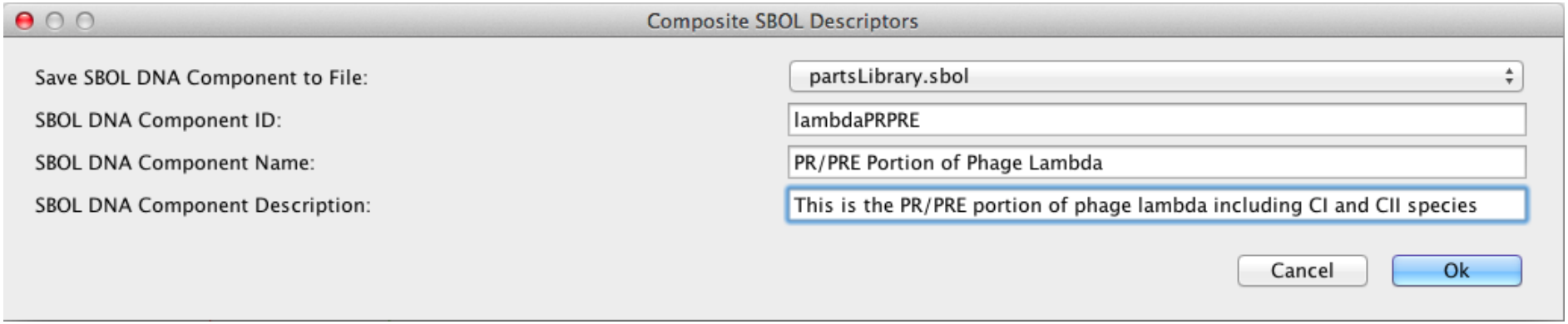
Associate SBOL Browser



Associate SBOL to the Model

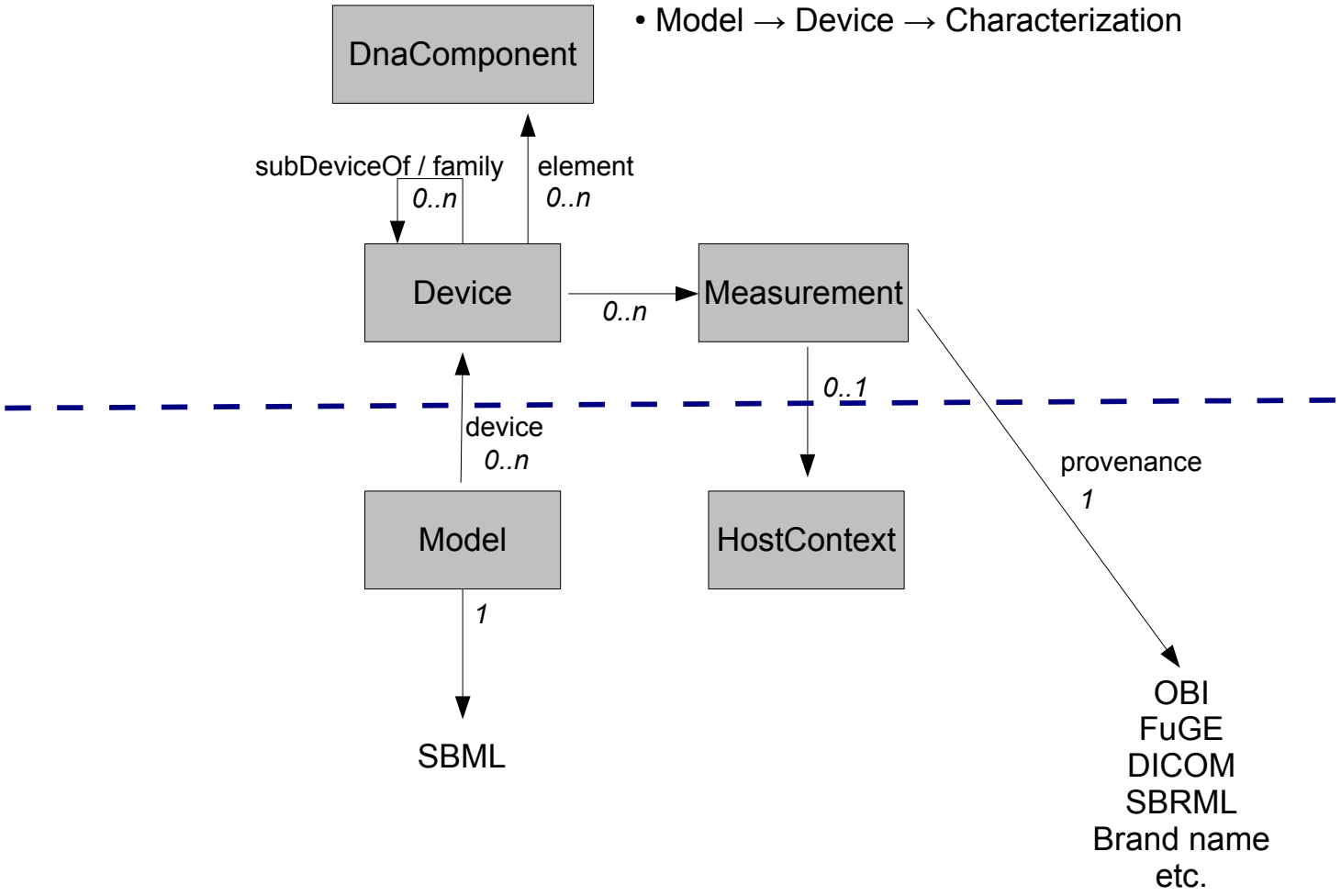


Composite SBOL Descriptors

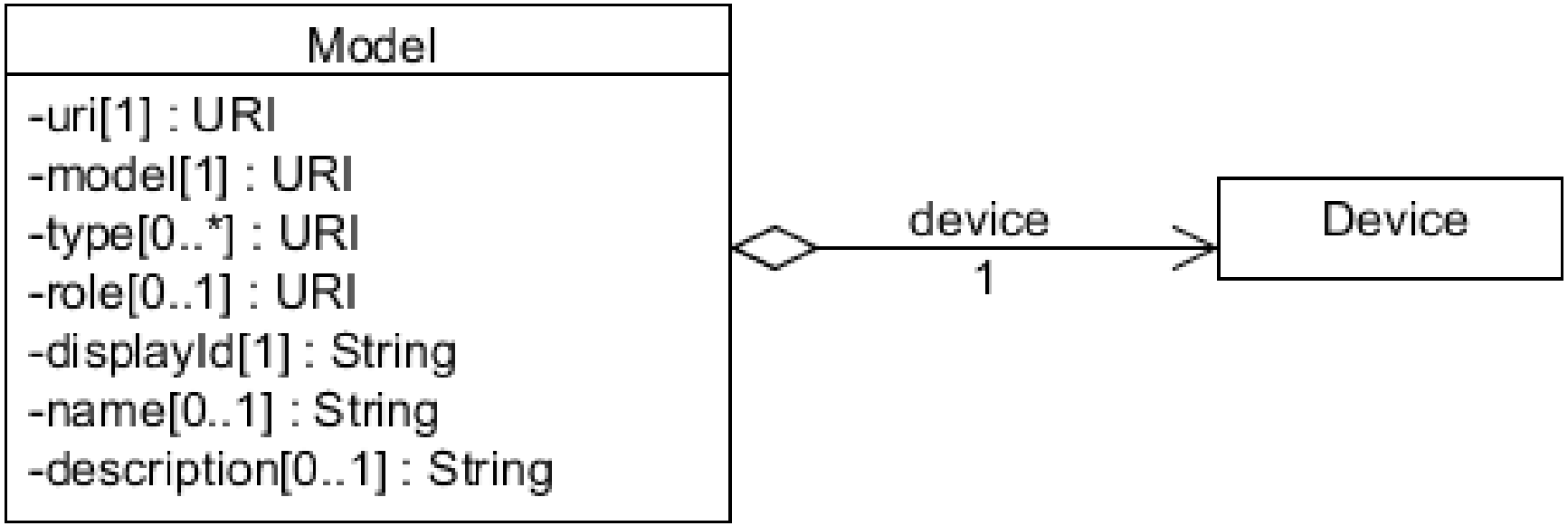


SBOL Extensions

Core idea
- Model → Device → DNA
- DNA → Device → Characterization
- Model → Device → Characterization



Proposal for a New Model Class



- The basic definition of this class is: “A Model is a linkage between a functional grouping of DNA components (a Device) and a mathematical and/or logical description of this group’s behavior (a model).”
- Referenced model must be written in a standardized modeling language such as the SBML or CellML.
- Type URIs reference terms from the *Systems Biology Ontology* (SBO).
- Role URIs?

Immediate Goals

- A user of the SBOL modeling extension should be able to:
  - Associate one or more models with a Device (in case there are multiple models that refine a Device's behavior or models that are written in competing standards).
  - Associate one or more Devices with a model (in case there is a model that templates the behavior for a class of Devices).
  - Document the type and role of a model such that said information can be obtained without having to parse the model.
- Also, a developer of the SBOL modeling extension should be able to change and update its data model without violating any expectations on the part of the Device data model.

Comments

- Should models be restricted to SBML only?
  - If so, change “model” to “sbmlFile”?
  - If not, how should the model class indicate the modeling language used?
- Should types of models be restricted to SBO terms?
- What is the difference between role and type?
- What is the connection between this extension and others such as regulatory or ports?