

Synthetic Biology Open Language (SBOL) Version 3.0

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Version 3.0

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1 Purpose

Synthetic biology builds upon genetics, molecular biology, and metabolic engineering by applying engineering principles to the design of biological systems. When designing a synthetic system, synthetic biologists need to exchange information about multiple types of molecules, the intended behavior of the system, and actual experimental measurements. Furthermore, there are often multiple aspects to a design such as a specified nucleic acid sequence (e.g., a sequence that encodes an enzyme or transcription factor), the molecular interactions that a designer intends to result from the introduction of this sequence (e.g., chemical modification of metabolites or regulation of gene expression), and the experiments and data associated with the system. All these perspectives need to be connected together to facilitate the engineering of biological systems.

The *Synthetic Biology Open Language* (SBOL) has been developed as a standard to support the specification and exchange of biological design information in synthetic biology, following an open community process involving both “wet” bench scientists and “dry” scientific modelers and software developers, across academia, industry, and other institutions. Previous nucleic acid sequence description formats lack key capabilities relative to SBOL, as shown in [Figure 1](#). Simple sequence encoding formats such as FASTA encode little besides sequence information. More sophisticated formats such as GenBank and Swiss-Prot provide a flat annotation of sequence features that is well suited to describing natural systems but unable to represent the functional relations and multi-layered design structure common to engineered systems. Modeling languages, such as the Systems Biology Markup Language (SBML) [Hucka et al. \(2003\)](#), can be used represent biological processes, but are not sufficient to represent the associated nucleotide or amino acid sequences. SBOL covers both of these needs, by providing a modular and hierarchical representation of the structure and function of a genetic design, as well as its relationship to and use within experiment plans, data, models, etc.

SBOL uses existing Semantic Web practices and resources, such as *Uniform Resource Identifiers* (URIs) and ontologies, to unambiguously identify and define biological system elements, and to provide serialization formats for encoding this information in electronic data files. The SBOL standard further describes the rules and best practices on how to use this data model and populate it with relevant design details. The definition of the data model, the rules on the addition of data within the format, and the representation of this in electronic data files are intended to make the SBOL standard a useful means of promoting data exchange between laboratories and between software programs.

Differences from Prior Versions of SBOL

SBOL 1 focused on representing the structural aspects of genetic designs: it allowed the exchange of information about DNA designs and their sequence features, but could not represent molecules other than DNA or the functional aspects of designs. SBOL 2 enabled the description and exchange of hierarchical, modular representations of both the intended structure and function of designed biological systems, as well as providing support for representing provenance, combinatorial designs, genetic design implementations, external file attachments, experimental data, and numerical measurements. SBOL 3.0, defined by this document, condenses and simplifies these prior representations based on experiences in deployment across a variety of scientific and industrial settings.

Specifically, SBOL 3.0 improves on its predecessor SBOL 2.3 by:

- Separating sequence features from part/sub-part relationships.
- Renaming ComponentDefinition/Component to Component/SubComponent.
- Merging Component and Module classes.
- Ensuring consistency between data model and ontology terms.
- Extending the means to define and reference SubComponents.
- Refining requirements on object URIs.

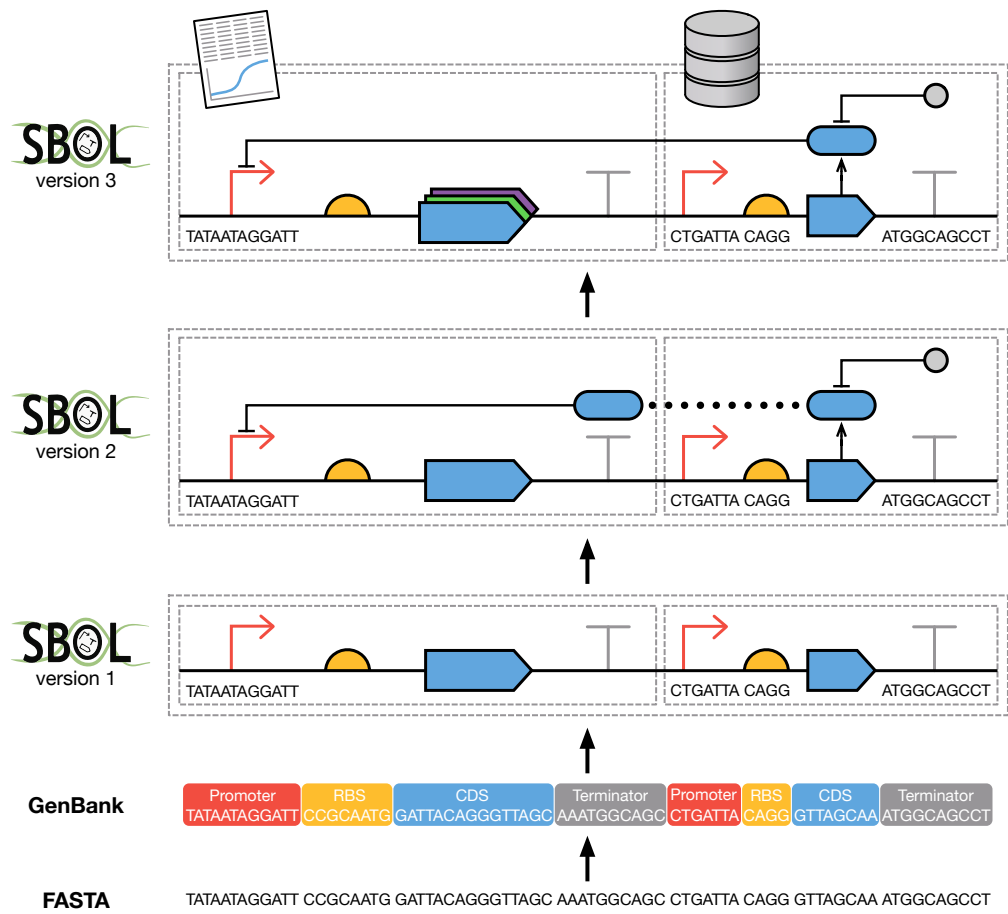


Figure 1: SBOL extends prior sequence description formats to represent both the structure and function of a genetic design in a modular, hierarchical manner, as well as its relationship to, and use within, experiments, plans, data, models, etc.

- Enabling graph-based serialization. 1
- Moving to Systems Biology Ontology (SBO) for Component types. 2
- Making all sequence associations explicit. 3
- Making interfaces explicit. 4
- Generalizing SequenceConstraints into a general structural Constraint class. 5
- Expanding the set of allowed sequence constraints. 6

2 A Brief History of SBOL

The SBOL effort was started in 2006 with the goal of developing a data exchange standard for genetic designs. Herbert Sauro (University of Washington) secured a grant from Microsoft in the field of computational synthetic biology, which was used to fund the initial meeting in Seattle on April 26-27, 2008. This workshop was organized by Herbert Sauro, Sean Sleight, and Deepak Chandran, and included talks by Raik Gruenberg, Kim de Mora, John Cumbers, Christopher Anderson, Mac Cowell, Jason Morrison, Jean Peccoud, Ralph Santos, Andrew Milar, Vincent Rouilly, Mike Hucka, Michael Blinov, Lucian Smith, Sarah Richardson, Guillermo Rodrigo, Jonathan Goler, and Michal Galdzicki.

Michal's early efforts were instrumental in making SBOL successful. As part of his doctoral work, he led the development of PoBol (Provisional BioBrick Language), as SBOL was originally known. He organized annual workshops from 2008 to 2011 and kept the idea of developing a genetic design standard alive. The original SBOL 1.0 was developed by a small group of dedicated researchers calling themselves the Synthetic Biology Data Exchange Working Group, meeting at Stanford in 2009 and Anaheim, CA in 2010. During the Anaheim meeting, the community decided to write a letter to Nature Biotechnology highlighting the issue of reproducibility in synthetic biology [Peccoud et al. \(2011\)](#). This letter was initiated by Jean Peccoud and submitted by participants of the Anaheim meeting, including Deepak Chandran, Douglas Densmore, Dmytriv, Michal Galdzicki, Timothy Ham, Cesar Rodriguez, Jean Peccoud, Herbert Sauro, and Guy-Bart Stan. The overall pace of development quickened when several new members joined at the next workshop in Blacksburg, Virginia on January 7-10, 2011. This early work was also supported by an STTR grant from the National Institute of Health (NIH #1R41LM010745 and #9R42HG006737, from 2010-13) in collaboration with Clark & Parsia, LLC (Co-PIs: John Gennari and Evren Sirin). New members included Cesar Rodriguez, Mandy Wilson, Guy-Bart Stan, Chris Myers, and Nicholas Roehner.

The SBOL Developers Group was officially established at a meeting in San Diego in June 2011. Rules of governance were established, and the first SBOL editors were elected: Mike Galdzicki, Cesar Rodriguez, and Mandy Wilson. At our next meeting in Seattle in January 2012, Herbert Sauro was elected the SBOL chair, and two new editors were added: Matthew Pocock and Ernst Oberortner. New developers joining at these workshops included several representatives from industry, Kevin Clancy, Jacob Beal, Aaron Adler, and Fusun Yaman Sirin. New members from Newcastle University included Anil Wipat, Matthew Pocock, and Goksel Misirli.

Development of the first software library (libSBOLj) based on the SBOL standard was initiated by Allan Kuchinsky, a research scientist from Agilent, at the 2011 meeting. By the time of the 2012 meeting, the first data exchange between software tools using SBOL was conducted when a design was passed from Newcastle University's VirtualParts Repository to Boston University's Eugene tool, and finally to University of Utah's iBioSim tool.

SBOL 1.0 was officially released in October 2011. In March 2012, SBOL 1.1 was released, the version that this document replaces. SBOL 1.1 did not make any major changes, but provided a number of small adjustments and clarifications, particularly around the annotation of sequences. Multi-institutional data exchange using SBOL 1.1 was later demonstrated in Nature Biotechnology [Galdzicki et al. \(2014\)](#).

While SBOL 1.1 had a number of significant advantages over the GenBank representation of DNA sequences, such as representing hierarchical organization of DNA components, it was still limited in other respects. The major topic of discussion at the 8th SBOL Workshop at Boston University in November 2012 was how to address these shortcomings through extensions. Several extensions were discussed at this meeting, such as a means to describe genetic regulation, which later became important classes in the current 2.x specification.

A general framework for SBOL 2.0 emerged at the 9th SBOL workshop at Newcastle University in April 2013. Subsequently, Nicholas Roehner, Matthew Pocock, and Ernst Oberortner drafted a proposal for SBOL 2.0, and Nicholas presented this proposal at the SEED conference in Los Angeles in July 2014 [Roehner et al. \(2015\)](#). The proposed 2.0 data model was discussed over the course of the 10th, 11th, and 12th workshops. The SBOL 2.0 specification document was drafted at the 13th workshop in Wittenberg, Germany. The SBOL 2.x data model presented was essentially the result of these meetings and ongoing discussions conducted through the SBOL Developers mailing lists, plus minor adjustments and updates approved by the community through subsequent

meetings and mailing list discussions.

From 2014 to 2019, development of SBOL 2.x was funded in large part by a grant from the National Science Foundation (DBI-1355909 and DBI-1356041). The SBOL 2.x specification documents and the supporting software libraries are due in no small part to this support. Any opinions, findings, and conclusions or recommendations expressed in SBOL materials are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

The Computational Modeling in Biology Network ([COMBINE](#)) holds regular workshops at which synthetic biologists and systems biologists work toward a common goal of integrating biological knowledge through interoperable and non-overlapping data standards. Several SBOL Developers proposed that SBOL join this larger standards community after attending a COMBINE workshop in April 2014. The proposal passed and SBOL workshops have been co-located with COMBINE meetings since the 11th workshop at the University of Southern California in August 2014.

In 2019 the SBOL Industrial Consortium was established as a pre-competitive non-profit organization supporting innovation, dissemination, and integration of SBOL standards, tools and practices for practical applications in an industrial environment. The SBOL Industrial Consortium meets regularly to coordinate its activities, and organises an Industrial Advisory Board to give an industrial perspective on SBOL, as well as providing financial support for projects, activities, and infrastructure within the SBOL community. Member organisations include Raytheon BBN Technologies, Doulix, Integrated DNA Technologies, Twist Bioscience, Amyris, Inscripta, Teselagen, Shipyard Toolchains, and Zymergen.

Discussions related to SBOL 3 began at the COMBINE meetings and on the mailing list beginning in the summer of 2018. Over the next year and a half, several SBOL Enhancement Proposals (SEPs) were written and discussed. During the early months of 2020, these SEPs were voted on and approved by the SBOL community. The initial version of the SBOL 3 specification was drafted during HARMONY 2020 at the European Bioinformatics Institute (EBI) in Hinxton, United Kingdom in March 2020.

The authors would also like to thank Michael Hucka for developing the LaTeX style file used to develop this document ([Hucka, 2017](#)).

3 Overview of SBOL

Synthetic biology designs can be described using:

- Structural terms, e.g., a set of annotated sequences or information about the chemical makeup of components.
- Functional terms, e.g., the way that components might interact with each other.

As an example, consider an expression cassette, such as the one found in the plasmid pUC18 [Norrander et al. \(1983\)](#). The system is designed to visually indicate whether a gene has been inserted into the plasmid: in the presence of IPTG, it expresses an enzyme that hydrolyses X-gal to form a blue product, but successful insertion disrupts the expression cassette and prevents the formation of this product. Internally, it has a number of parts, including a promoter, the lac repressor binding site, and the lacZ coding sequence. These parts have specific component-level interactions with IPTG and X-gal, as well as native host gene products, transcriptional machinery, and translational machinery that collectively cause the desired system-level behavior.

In SBOL 3, both the structural and functional aspects are described using a class called **Component**, as depicted in [Figure 2](#). Namely, to represent structural aspects, a **Component** can include **Features**, some of which may be at some **Location** within a **Sequence**. A **Component** can also include **Constraints** between these features. To represent functional aspects, a **Component** can include **Interactions** that can refer to relationships between participating **Features**. Finally, a **Component** can have its behavior described using a **Model**.

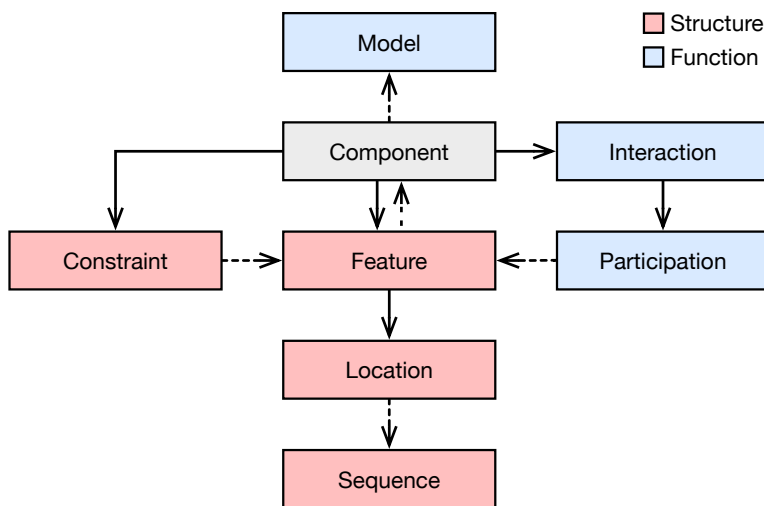


Figure 2: The SBOL **Component** object and related objects. Solid arrows indicates ownership, whereas a dashed arrow represents a reference to an object of another class. Red boxes represent structural objects, while blue boxes represent functional objects. To represent structural aspects, a **Component** can include **Features**, which may refer to **Locations** within a **Sequence**. A **Component** can also include **Constraints** between these features. To represent functional aspects, a **Component** can include **Interactions** that can refer to relationships between participating **Features**. Finally, a **Component** can have its behavior described using a **Model**.

To continue with the pUC18 example, the description would begin with a top-level **Component** that represents the entire system. This **Component** specifies the structural elements that make up the cassette by referencing a number of **SubComponent** objects. These would include the DNA **SubComponent** for the promoter and the simple chemical **SubComponent** for IPTG, for example. The **Component** objects can be organized hierarchically. For example, the plasmid **Component** might reference **SubComponents** for the promoter, coding sequence, etc. Each **Component** object

can also include the actual [Sequence](#) information (if available), as well as [SubComponent](#) objects that identify the [Locations](#) of the promoters, coding sequences, etc., on the [Sequence](#). In order to specify functional information, the [Component](#) can also specify [Interaction](#) objects that describe any qualitative relationships among [SubComponent Participations](#), such as how IPTG and X-gal interact with the gene products. Finally, a [Component](#) object can point to a [Model](#) object that provides a reference to a complete computational model expressed in a language such as SBML [Hucka et al. \(2003\)](#), CellML [Cuellar et al. \(2003\)](#), or MATLAB [MathWorks \(2015\)](#).

Whereas [Figure 2](#) provides an overview of the classes used for describing designs within the SBOL 3 data model, [Figure 3](#) shows the rest of the classes used to describe the usage of a design within design-build-test-learn workflows in general. In particular, designs can be expressed using [CombinatorialDerivations](#), [Components](#), and [Sequences](#). These can describe not only genetic designs, but also designs for strains, multicellular systems, media, samples, etc. A [CombinatorialDerivation](#) allows one to specify a design pattern where individual [SubComponents](#) can be selected from a set of variants. The [Implementation](#) class is the build class, and it is used to represent physical artifacts like an actual sample of a plasmid. The [Experiment](#) and [ExperimentalData](#) classes are the test classes, allowing description of a collection of data generated in an experiment. The [Model](#) class, discussed earlier, associates learned information with a design. The [prov:Activity](#) class is taken from the provenance ontology (PROV-O), which is described in [Section A.1](#). For example, a build [prov:Activity](#) describes how an [Implementation](#) is constructed using a [Component](#) description. On the other hand, a test [prov:Activity](#) describes how an [Experiment](#) is conducted using an [Implementation](#) artifact. The [Collection](#) class has members, which can be of any of these types or [Collections](#) themselves. Finally, all of these objects can refer to objects of the [Attachment](#) class, which are used to link out to external data (images, spreadsheets, textual documents, etc.). The next sections provide complete definitions and details for all of these classes.

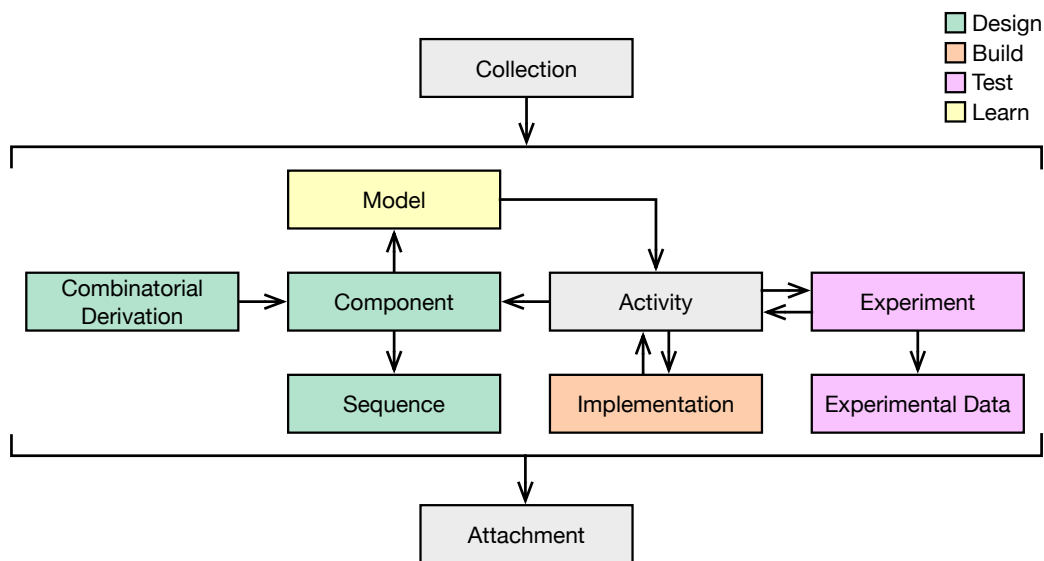


Figure 3: Main classes of information represented by the SBOL 3 standard, and their relationships. Green boxes represent design classes, orange boxes represent build classes, purple boxes represent test classes, yellow boxes represent learn classes, and the gray boxes represent additional utility classes. Each of these classes will be described in more detail below.

4 Conventions

This section provides some preliminary information to aid in the understanding of the specification. The SBOL data model is specified using Unified Modeling Language (UML) 2.0 diagrams (OMG 2005). This section reviews terminology conventions, the basics of UML diagrams, and our naming conventions.

4.1 Terminology Conventions

This document indicates requirement levels using the controlled vocabulary specified in IETF RFC 2119. In particular, the key words “MUST”, “MUST NOT”, “REQUIRED”, “SHALL”, “SHALL NOT”, “SHOULD”, “SHOULD NOT”, “RECOMMENDED”, “MAY”, and “OPTIONAL” in this document are to be interpreted as described in RFC 2119.

- The words “MUST”, “REQUIRED”, or “SHALL” mean that the item is an absolute requirement.
- The phrases “MUST NOT” or “SHALL NOT” mean that the item is an absolute prohibition.
- The word “SHOULD” or the adjective “RECOMMENDED” mean that there might exist valid reasons in particular circumstances to ignore a particular item, but the full implications need to be understood and carefully weighed before choosing a different course.
- The phrases “SHOULD NOT” or “NOT RECOMMENDED” mean that there might exist valid reasons in particular circumstances when the particular behavior is acceptable or even useful, but the full implications needs to be understood and the case carefully weighed before implementing any behavior described with this label.
- The word “MAY” or the adjective “OPTIONAL” mean that an item is truly optional.

4.2 UML Diagram Conventions

The types of biological design data modeled by SBOL are commonly referred to as *classes*, especially when discussing the details of software implementation. Each SBOL class can be instantiated by many SBOL objects. These objects MAY contain data that differ in content, but they MUST agree on the type and form of their data as dictated by their common class. Classes are represented in UML diagrams as rectangles labeled at the top with class names (see Figure 4 for examples).

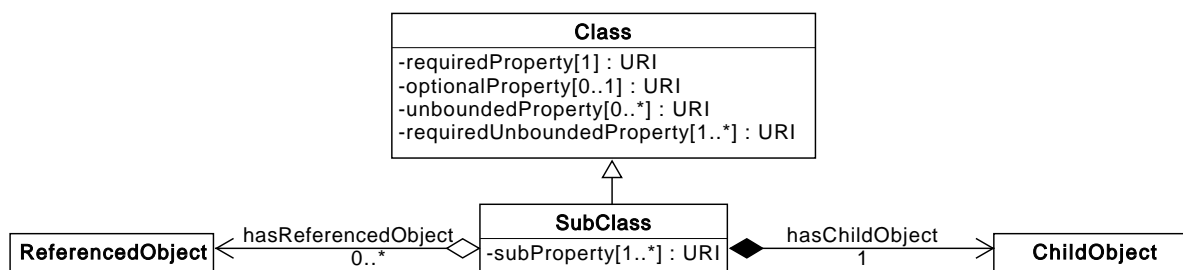


Figure 4: Examples of UML diagram conventions used in this document

Classes can be connected to other classes by association properties, which are represented in UML diagrams as arrows. These arrows are labeled with data cardinalities in order to indicate how many values a given association

property can possess (see below). The remaining (non-association) properties of a class are listed below its name. Each of the latter properties is labeled with its data type and cardinality.

In the case of an association property, the class from which the arrow originates is the owner of the association property. A diamond at the origin of the arrow indicates the type of association. Open-faced diamonds indicate shared aggregation, also known as a reference, in which the owner of the association property exists independently of its value.

By contrast, filled diamonds indicate composite aggregation, also known as a part-whole relationship, in which the value of the association property **MUST NOT** exist independently of its owner. In addition, in the SBOL data model, it is **REQUIRED** that the value of each composite aggregation property is a unique SBOL object (that is, not the value for more than one such property). Note that in all cases, composite aggregation is used in such a way that there **SHOULD NOT** be duplication of such objects. Such objects are also commonly referred to as “child” objects, and their owning objects as “parent” objects.

All SBOL properties are labeled with one of several restrictions on data cardinality. These are:

- 1 - **REQUIRED**, one: there **MUST** be exactly one value for this property.
- 0...1 - **OPTIONAL**: there **MAY** be a single value for this property, or it **MAY** be absent.
- 0...* - **unbounded**: there **MAY** be any number of values for this property, including none.
- 1...* - **REQUIRED**, unbounded: there **MAY** be any number of values for this property, as long as there is at least one.
- *n*...* - **at least**: there **MUST** be at least *n* values for this property.

Finally, classes can inherit the properties of other classes. Inheritance relationships are represented in UML diagrams as open-faced, triangular arrows that point from the inheriting class to the inherited class. Some classes in the SBOL data model cannot be instantiated as objects and exist only to group common properties for inheritance. These classes have italicized names and are known as abstract classes.

4.3 Naming and Typographic Conventions

SBOL classes are named using upper “camel case,” meaning that each word is capitalized and all words are run together without spaces, e.g., **Identified**, **SequenceFeature**. Properties, on the other hand, are named using lower camel case, meaning that they begin lowercase (e.g., **role**) but if they consist of multiple words, all words after the first begin with an uppercase letter (e.g., **roleIntegration**). SBOL properties are always given singular names irrespective of their cardinality, e.g., **role** is used rather than **roles** even though a component can have multiple roles. This is because each relation can potentially stand on its own, irrespective of the existence of others in the set.

5 Identifiers and Primitive Types

5.1 Uniform Resource Identifiers

As SBOL is built upon the Resource Description Framework (RDF), all class instances are identified by a Uniform Resource Identifier (URI). In the SBOL data model, the value of an association property MUST be a URI or set of URIs that refer to SBOL objects belonging to the class at the tip of the arrow. Every **Identified** object's URI MUST be globally unique among all other **Identified** object URIs. It is also highly RECOMMENDED that the URI structure follows the recommended best practices for compliant URIs specified in [Section 7.2](#).

Whenever a **TopLevel** object's URI is a URL (e.g., following the conventions of HTTP(S) rather than a UUID), its structure MUST comply with the following rules:

- A **TopLevel** URL MUST use the following pattern: `[namespace]/[local]/[displayId]`, where **namespace** and **displayId** are required fragments, and the **local** fragment is an optional relative path. For example, a **Component** might have the URL `https://synbiohub.org/public/igem/BBa_J23070`, where **namespace** is `https://synbiohub.org`, **local** is `public/igem`, and **displayId** is `BBa_J23070`.
- A **TopLevel** object's URL MUST NOT be included as prefix for any other **TopLevel** object (except for its controlling **Namespace**). For example, the `BBa_J23070_seq` **Sequence** object cannot have a URL of `https://synbiohub.org/public/igem/BBa_J23070/BBa_J23070_seq`, since the `https://synbiohub.org/public/igem/BBa_J23070` prefix is already used as a URL for the `BBa_J23070` **Component** object.
- The URL of any child or nested object MUST use the following pattern: `[parent]/[displayId]`, where **parent** is the URL of its parent object. Multiple layers of child objects are allowed using the same `[parent]/[displayId]` pattern recursively. For example, a **SequenceFeature** object owned by the `BBa_J23070` **Component** and having a **displayId** of `annotation1` will have a URL of `https://synbiohub.org/public/igem/BBa_J23070/annotation1`. Similarly, the `loc1` **Location** child of the `annotation1` **SequenceFeature** object will have the URL `https://synbiohub.org/public/igem/BBa_J23070/annotation1/loc1`.

5.2 Primitive Data Types

When SBOL uses simple “primitive” data types such as **Strings** or **Integers**, these are defined as the following specific formal types:

- **String**: <http://www.w3.org/TR/xmlschema11-2/#string>
Example: “LacI coding sequence”
- **Integer**: <http://www.w3.org/TR/xmlschema11-2/#integer>
Example: 3
- **Long**: <http://www.w3.org/TR/xmlschema11-2/#long>
Example: 9223372036854775806
- **Double**: <http://www.w3.org/TR/xmlschema11-2/#double>
Example: 3.14159
- **Boolean**: <http://www.w3.org/TR/xmlschema11-2/#boolean>
Example: true

The term **literal** is used to denote an object that can be any of the five types listed above.

In addition to the simple types listed above, SBOL also uses objects with types *Uniform Resource Identifier* ([URI](#)). It is important to realize that in RDF, a [URI](#) might or might not be a resolvable URL (web address). A [URI](#) is always a globally unique identifier within a structured namespace. In some cases, that name is also a reference to (or within) a document, and in some cases that document can also be retrieved (e.g., using a web browser).

1
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6 SBOL Data Model

The section describes the SBOL data model in detail. Best practices when using the standard can be found in [Section 7](#).

6.1 Identified

All SBOL-defined classes are directly or indirectly derived from the [Identified](#) abstract class. This inheritance means that all SBOL objects are uniquely identified using [URIs](#) that uniquely refer to these objects within an SBOL document or at locations on the World Wide Web.

As shown in [Figure 5](#), the [Identified](#) class includes the following properties: [displayId](#), [name](#), [description](#), [prov:wasDerivedFrom](#), and [prov:wasGeneratedBy](#).

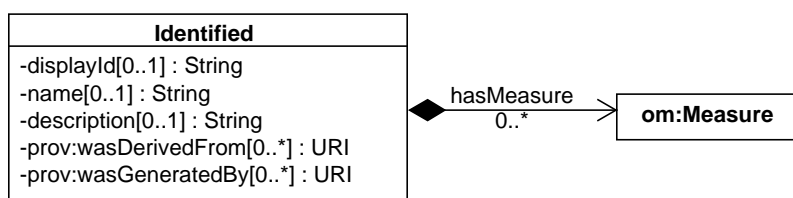


Figure 5: Diagram of the [Identified](#) abstract class and its associated properties

The [displayId](#) property

The [displayId](#) property is an OPTIONAL identifier with a data type of [String](#). This property is intended to be an intermediate between a URI and the [name](#) property that is machine-readable, but more human-readable than the full URI of an object.

If the [displayId](#) property is used, then its [String](#) value MUST be composed of only alphanumeric or underscore characters and MUST NOT begin with a digit.

Note that for objects whose URI is a URL, the requirements on URL structure in [Section 5.1](#) imply that the [displayId](#) MUST be set.

The [name](#) property

The [name](#) property is OPTIONAL and has a data type of [String](#). This property is intended to be displayed to a human when visualizing an [Identified](#) object.

If an [Identified](#) object lacks a name, then software tools SHOULD instead display the object's [displayId](#) or URI. It is RECOMMENDED that software tools give users the ability to switch perspectives between [name](#) properties that are human-readable and [displayId](#) properties that are less human-readable, but are more likely to be unique.

The [description](#) property

The [description](#) property is OPTIONAL and has a data type of [String](#). This property is intended to contain a more thorough text description of an [Identified](#) object.

The [prov:wasDerivedFrom](#) property

An [Identified](#) object can have zero or more [prov:wasDerivedFrom](#) properties, each of type URI. This property is defined by the PROV-O ontology and is located in the <https://www.w3.org/TR/prov-o/> namespace (Reference:

Section A.1).

An SBOL object with this property refers to one or more SBOL objects or non-SBOL resources from which this object was derived. An SBOL object MUST NOT refer to itself via its own `prov:wasDerivedFrom` property or form a cyclical chain of references via its `prov:wasDerivedFrom` property and those of other SBOL objects. For example, the reference chain “A was derived from B and B was derived from A” is cyclical.

The `prov:wasGeneratedBy` property

An `Identified` object can have zero or more `prov:wasGeneratedBy` properties, each of type URI. This property is defined by the PROV-O ontology and is located in the <https://www.w3.org/TR/prov-o/> namespace (Reference: Section A.1).

An SBOL object with this property refers to one or more `prov:Activity` objects that describe how this object was generated. Provenance history formed by `prov:wasGeneratedBy` properties of `Identified` objects and entity references in `prov:Usage` objects MUST NOT form circular reference chains.

The `hasMeasure` property

An `Identified` object can have zero or more `hasMeasure` properties, each of type URI. This property is defined by the OM ontology and is located in the <http://www.ontology-of-units-of-measure.org/resource/om-2/> namespace (Reference: Section A.2).

An SBOL object with this property refers to one or more `om:Measure` objects that describe measured parameters for this object.

6.2 TopLevel

`TopLevel` is an abstract class that is extended by any `Identified` class that can be found at the top level of an SBOL document or file. In other words, `TopLevel` objects are not nested inside any other object via *composite aggregation* (represented by a filled diamond arrowhead on the UML diagrams). Instead of nesting, composite `TopLevel` objects refer to subordinate `TopLevel` objects by their URIs using *shared aggregation* (represented by an open-faced/non-filled diamond arrowhead on the UML diagrams). The `TopLevel` classes defined in this specification are `Sequence`, `Component`, `Model`, `Collection`, `CombinatorialDerivation`, `Implementation`, `Attachment`, `ExperimentalData`, `prov:Activity`, `prov:Agent`, `prov:Plan` (see Figure 6). Each of these classes is described in more detail below, except for the classes from the provenance ontology (PROV-O), which are described in Section A.1.

The `hasAttachment` property

A `TopLevel` object can have zero or more `hasAttachment` properties, each of type URI specifying an `Attachment` object. The `Attachment` class is described in more detail in Section 6.10.

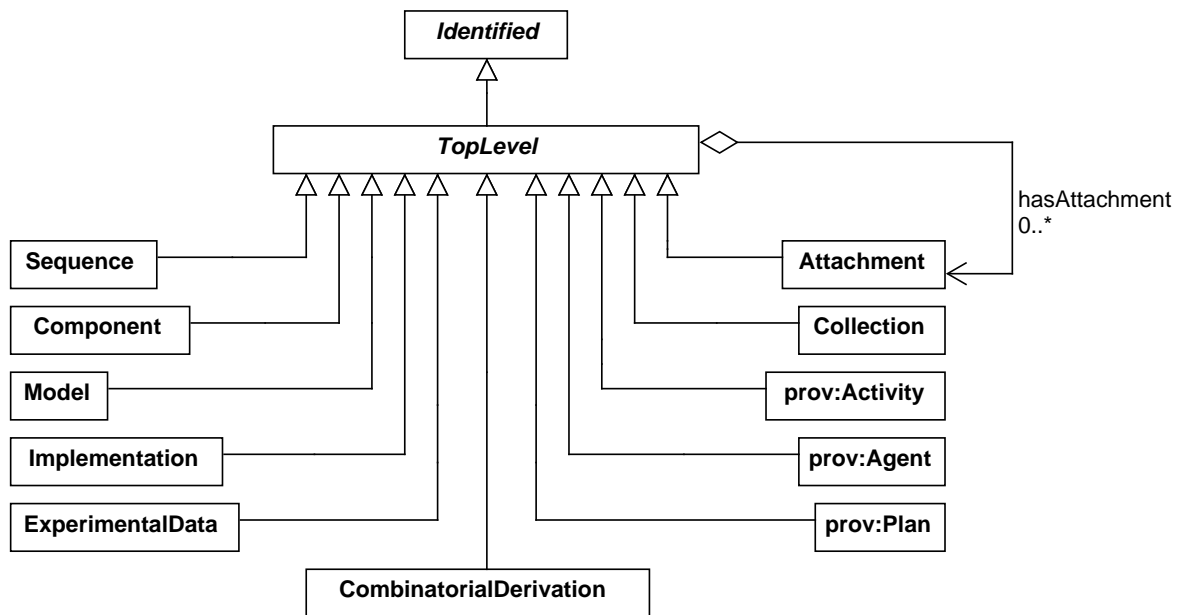
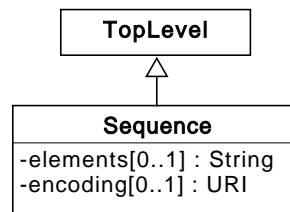
6.3 Sequence

The purpose of the `Sequence` class is to represent the primary structure of a `Component` object and the manner in which it is encoded. This representation is accomplished by means of the `elements` property and `encoding` property (Figure 7).

The `elements` property

The `elements` property is an OPTIONAL `String` of characters that represents the constituents of a biological or chemical molecule. For example, these characters could represent the nucleotide bases of a molecule of DNA, the amino acid residues of a protein, or the atoms and chemical bonds of a small molecule.

If the `elements` property is not set, then it means the particulars of this `Sequence` have not yet been determined.

Figure 6: Classes that inherit from the `TopLevel` abstract class.Figure 7: Diagram of the `Sequence` class and its associated properties.

The `encoding` property

The `encoding` property has a data type of `URI`, and is OPTIONAL unless `elements` is set, in which case it is REQUIRED. This property MUST indicate how the `elements` property of a `Sequence` are formed and interpreted.

For example, the `elements` property of a `Sequence` with an IUPAC DNA encoding property MUST contain characters that represent nucleotide bases, such as a, t, c, and g. The `elements` property of a `Sequence` with a Simplified Molecular-Input Line-Entry System (SMILES) encoding, on the other hand, MUST contain characters that represent atoms and chemical bonds, such as C, N, O, and =.

Table 1 provides a list of possible `URI` values for the `encoding` property. The terms in Table 1 are organized by the type of `Component` (see Table 2) that typically refer to a `Sequence` with such an `encoding`. It is RECOMMENDED that the encoding property of a `Sequence` contains a `URI` from Table 1. When the `encoding` of a `Sequence` is well described by one of the `URIs` in Table 1, it MUST contain that `URI`.

More information on IUPAC encoding can be found at <http://www.bioinformatics.org/sms2/iupac.html>.

Encoding	URI	Component Type
IUPAC DNA, RNA	http://sbols.org/v3#iupacNucleicAcid	DNA, RNA
IUPAC Protein	http://sbols.org/v3#iupacAminoAcid	Protein
SMILES	http://www.opensmiles.org/opensmiles.html	Simple Chemical

Table 1: URIs for specifying the **encoding** property of a **Sequence**, organized by the type of **Component** (see Table 2) that typically refer to a **Sequence** with such an **encoding**.

6.4 Component

The **Component** class represents the structural and/or functional entities of a biological design. The primary usage of this class is to represent entities with designed sequences, such as DNA, RNA, and proteins, but it can also be used to represent any other entity that is part of a design, such as simple chemicals, molecular complexes, strains, media, light, and abstract functional groupings of other entities.

As shown in Figure 8, the **Component** class describes a design entity using the following properties: **type**, **role**, **hasSequence**, **hasFeature**, **hasConstraint**, **hasInteraction**, **hasInterface**, and **hasModel**. The **hasSequence**, **hasFeature**, and **hasConstraint** properties are used to represent structural information, while the **hasInteraction**, **hasInterface**, and **hasModel** are used to represent functional information.

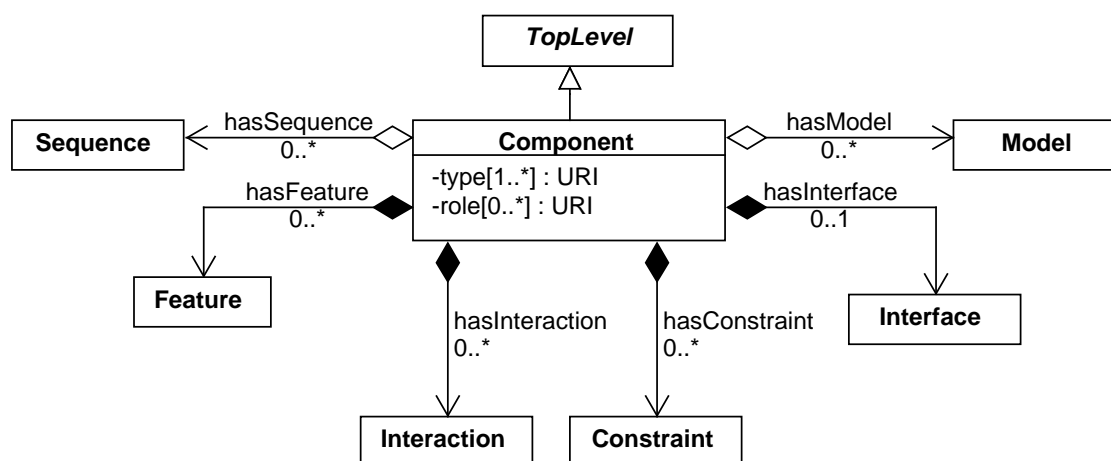


Figure 8: Diagram of the **Component** class and its associated properties.

The **type** property

A **Component** is REQUIRED to have one or more **type** properties, each of type **URI** specifying the category of biochemical or physical entity (for example DNA, protein, or simple chemical) that a **Component** object abstracts for the purpose of engineering design. For DNA or RNA entities, additional **type** properties MAY be used to describe nucleic acid topology (circular / linear) and strandedness (double- or single-stranded).

The **type** properties of every **Component** MUST include one or more **URI**s that MUST identify terms from appropriate ontologies, such as the physical entity representation branch of the Systems Biology Ontology Courtot et al. (2011) or the ontology of Chemical Entities of Biological Interest (ChEBI) Degtyarenko et al. (2008). In order to maximize the compatibility of designs, the **type** property of a **Component** SHOULD contain a **URI** from the physical entity representation branch of the Systems Biology Ontology Courtot et al. (2011). Table 2 provides a partial list of ontology terms and their **URI**s, and any **Component** that can be well-described by one of the terms in Table 2 MUST

use the [URI](#) for that term as a [type](#). Finally, if the [type](#) property contains multiple [URIs](#), then they MUST identify non-conflicting terms (otherwise, it might not be clear how to interpret them). For example, the SBO terms provided by [Table 2](#) would conflict because they specify classes of biochemical entities with different molecular structures.

Component Type	URI for SBO Term
DNA (Deoxyribonucleic acid)	https://identifiers.org/SBO:0000251
RNA (Ribonucleic acid)	https://identifiers.org/SBO:0000250
Protein (Polypeptide chain)	https://identifiers.org/SBO:0000252
Simple Chemical	https://identifiers.org/SBO:0000247
Non-covalent complex	https://identifiers.org/SBO:0000253
Functional Entity	https://identifiers.org/SBO:0000241

Table 2: Partial list of the most common SBO terms to specify the molecule type using the [type](#) property of a [Component](#). Systems of multiple interacting molecules (e.g., a plasmid expressing a protein) should use the functional entity type.

Nucleic Acid Topology types

Any [Component](#) classified as DNA (see [Table 2](#)) is RECOMMENDED to encode circular/linear topology information in an additional [type](#) field. This (topology) [type](#) field SHOULD specify a URI from the Topology Attribute branch of the Sequence Ontology (SO): this is currently just ‘linear’ or ‘circular’ as given in [Table 3](#). Topology information SHOULD be specified for DNA [Component](#) records with a fully specified sequence, except in three scenarios: if the DNA record does not have sequence information, or if the DNA record has incomplete sequence information, or if topology is genuinely unknown. For any [Component](#) classified as RNA (see [Table 2](#)), a topology type field is OPTIONAL. The default assumption in this case is linear topology. In any case, conflicting topologies MUST NOT be specified.

Any [Component](#) classified as DNA or RNA MAY also have strand information encoded in an additional (third) type field using a URI from the Strand Attribute branch of the SO (currently there are only two possible terms for single or double-stranded nucleic acids, given in [Table 3](#)). In absence of this field, the default strand information assumed for DNA is ‘double-stranded’ and for RNA is ‘single-stranded’.

Any other type of [Component](#) record (protein, simple chemical, etc.) SHOULD NOT have any type field pointing to SO terms from the topology or strand attribute branches of SO.

Note that a *circular* topology instructs software to interpret the beginning / end position of a given sequence (be it DNA or RNA) as arbitrary, meaning that sequence features MAY be mapped or identified across this junction. *Double stranded* instructs software to apply sequence searches to both strands (i.e., sequence and reverse complement of sequence).

Nucleic Acid Topology	URI for Nucleic Acid Topology Term in SO
linear	http://identifiers.org/so/SO:0000987
circular	http://identifiers.org/so/SO:0000988
single-stranded	http://identifiers.org/so/SO:0000984
double-stranded	http://identifiers.org/so/SO:0000985

Table 3: Sequence Ontology (SO) terms to encode DNA or RNA topology information in the [type](#) properties of a [Component](#).

The *role* property

A **Component** MAY have any number of **role** properties, each of type **URI**, that MUST identify terms from ontologies that are consistent with the **type** property of the **Component**. For example, the **role** property of a DNA or RNA **Component** could contain URIs identifying terms from the Sequence Ontology (SO). As a best practice, a DNA or RNA **Component** SHOULD contain exactly one **URI** that refers to a term from the sequence feature branch of the SO. Similarly, the role properties of a protein and simple chemical **Component** SHOULD respectively contain **URIs** identifying terms from the **MolecularFunction** (GO:0003674) branch of the Gene Ontology (GO) and the **role** (CHEBI:50906) branch of the CHEBI ontology. Table 4 contains a partial list of possible ontology terms for the **role** properties and their **URIs**. These terms are organized by the type of **Component** to which they SHOULD apply (see Table 2). Any **Component** that can be well-described by one of the terms in Table 4 MUST use the **URI** for that term as a **role**.

These **URIs** might identify descriptive biological roles, such as “metabolic pathway” and “signaling cascade,” but they can also identify “logical” roles, such as “inverter” or “AND gate”, or other abstract roles for describing the function of design. Interpretation of the meaning of such roles currently depends on the software tools that read and write them.

Component Role	URI for Ontology Term	Component Type
Promoter	http://identifiers.org/so/SO:0000167	DNA
RBS	http://identifiers.org/so/SO:0000139	DNA
CDS	http://identifiers.org/so/SO:0000316	DNA
Terminator	http://identifiers.org/so/SO:0000141	DNA
Gene	http://identifiers.org/so/SO:0000704	DNA
Operator	http://identifiers.org/so/SO:0000057	DNA
Engineered Gene	http://identifiers.org/so/SO:0000280	DNA
mRNA	http://identifiers.org/so/SO:0000234	RNA
Effector	http://identifiers.org/chebi/CHEBI:35224	Small Molecule
Transcription Factor	http://identifiers.org/go/GO:0003700	Protein

Table 4: Partial list of ontology terms to specify the **role** property of a **Component**, organized by the type of **Component** to which they are intended to apply (see Table 2).

The *hasSequence* property

A **Component** MAY have any number of **hasSequence** properties, each of type **URI**, that MUST reference a **Sequence** object (see Section 6.3). These objects define the primary structure or structures of the **Component**.

If a **Feature** of a **Component** refers to a **Location**, and this **Location** refers to a **Sequence**, then the **Component** MUST also include a **hasSequence** property that refers to this **Sequence**.

Many **Component** objects will have exactly one **hasSequence** property that refers to a **Sequence** object. In this case, if its has a **type** from Table 2 and there is an **encoding** that is cross-listed with this term in Table 1, then the **Sequence** objects MUST have this encoding (e.g., a **Component** of **type** DNA must have a **Sequence** with an IUPAC DNA **encoding**). This **Sequence** is implicitly the entire sequence for this **Component** (In other words, it is equivalent to a **SequenceFeature** with an **EntireSequence Location** that refers to this **Sequence**).

The *hasFeature* property

A **Component** MAY have any number of **hasFeature** properties, each of type **URI** that MUST reference a **Feature** object (see Section 6.4.1). The set of relations between **Feature** and **Component** objects MUST be strictly acyclic.

Taking the **Component** class as analogous to a blueprint or specification sheet for a biological part or a system of interacting biological elements, the **Feature** class represents the specific occurrence of a part, subsystem, or other

notable aspect within that design. This mechanism also allows a biological design to include multiple instances of a particular part (defined by reference to the same [Component](#)). For example, the [Component](#) of a polycistronic gene could contain two [SubComponent](#) objects that refer to the same [Component](#) of a CDS. As another example, consider the [Component](#) for a network of two-input repressor devices in which the particular repressors have not yet been chosen. This [Component](#) could contain multiple [SubComponent](#) objects that refer to the same [Component](#) of an abstract two-input repressor device.

The [hasFeature](#) properties of [Component](#) objects can be used to construct a hierarchy of [SubComponent](#) and [Component](#) objects. If a [Component](#) in such a hierarchy refers to a [Location](#) object, and there exists a [Component](#) object lower in the hierarchy that refers to a [Location](#) object that refers to the same [Sequence](#) with the same [encoding](#), then the [elements](#) properties of these [Sequence](#) objects SHOULD be consistent with each other, such that well-defined mappings exist from the “lower level” [elements](#) to the “higher level” [elements](#) in accordance with their shared [encoding](#) properties. This mapping is also subject to any restrictions on the positions of the [Feature](#) objects in the hierarchy that are imposed by the [SubComponent](#), [SequenceFeature](#), or [Constraint](#) objects contained by the [Component](#) objects in the hierarchy.

For example, in a plasmid [Component](#) with a promoter [SubComponent](#), the sequence at the promoter's [Location](#) within the plasmid should be the sequence for the promoter. More concretely, consider DNA [Component](#) that refers to a [Sequence](#) with an IUPAC DNA [encoding](#) and an [elements](#) String of “gattaca.” In turn, this [Component](#) could contain a [SubComponent](#) that refers to a “lower level” [Component](#) that also refers to a [Sequence](#) with an IUPAC DNA [encoding](#). Consequently, a consistent [elements](#) String of this “lower level” [Sequence](#) could be “gatta,” or perhaps “tgta” if the [SubComponent](#) is positioned by a [Location](#) with an [orientation](#) of “reverse complement” (see [Section 6.4.2](#)).

The hasConstraint property

A [Component](#) MAY have any number of [hasConstraint](#) properties, each of type [URI](#), that MUST reference a [Constraint](#) object (see [Section 6.4.3](#)). These objects describe, among other things, any restrictions on the relative, sequence-based positions and/or orientations of the [Feature](#) objects contained by the [Component](#), as well as spatial relations such as containment and identity relations. For example, the [Component](#) of a gene might specify that the position of its promoter [SubComponent](#) precedes that of its CDS [SubComponent](#). This is particularly useful when a [Component](#) lacks a [Sequence](#) and therefore cannot specify the precise, sequence-based positions of its [SubComponent](#) objects using [Location](#) objects.

The hasInteraction property

A [Component](#) MAY have any number of [hasInteraction](#) properties, each of type [URI](#), that MUST reference an [Interaction](#) object (see [Section 6.4.4](#)).

The [Interaction](#) class provides an abstract, machine-readable representation of behavior within a [Component](#) (whereas a more detailed model of the system might not be suited to machine reasoning, depending on its implementation). Each [Interaction](#) contains [Participation](#) objects that indicate the roles of the [Feature](#) objects involved in the [Interaction](#).

The hasInterface property

A [Component](#) MAY have zero or one [hasInterface](#) property of type [URI](#) that MUST reference an [Interface](#) object (see [Section 6.4.5](#)).

An [Interface](#) object indicates the inputs, outputs, and non-directional points of connection to a [Component](#).

The hasModel property

A [Component](#) MAY have any number of [hasModel](#) properties, each of type [URI](#), that MUST reference a [Model](#) object (see [Section 6.8](#)).

[Model](#) objects are placeholders that link [Component](#) objects to computational models of any format. A [Component](#)

object can link to more than one [Model](#) since each might encode system behavior in a different way or at a different level of detail.

6.4.1 Feature

The [Feature](#) class, as shown in [Figure 9](#) is used to compose [Component](#) objects into a structural or functional hierarchy.

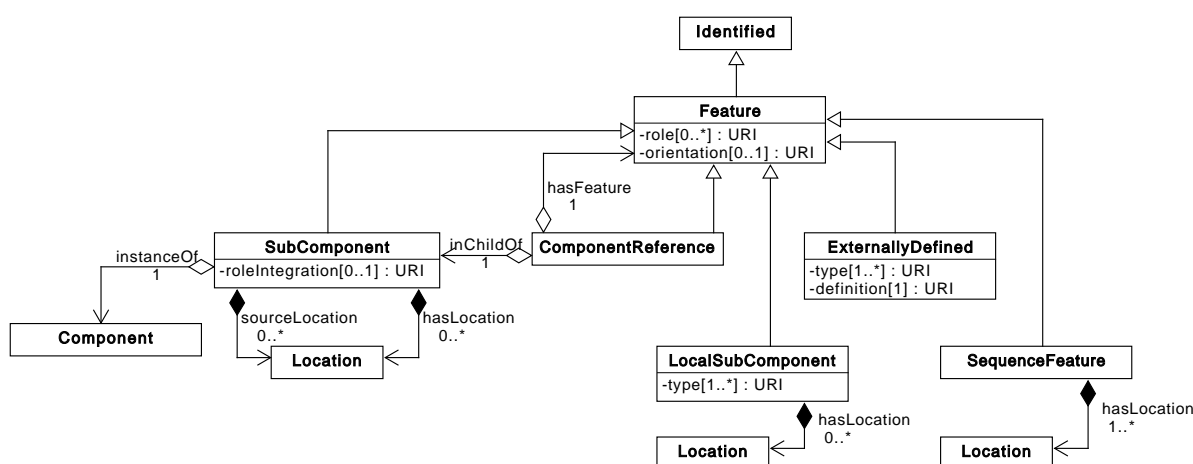


Figure 9: Diagram of the [Feature](#) class, its children, and associated properties.

The role property

Each [Feature](#) can have zero or more [role](#) property [URI](#)s describing the purpose or potential function of this [Feature](#) in the *context* of its parent [Component](#). If the [role](#) for a [SubComponent](#) is left unspecified, then the [role](#) is determined by the [role](#) property of the [Component](#) that it is an `instanceOf`. If provided, these [role](#) property [URI](#)s MUST identify terms from appropriate ontologies. Roles are not restricted to describing biological function; they may annotate a [Feature](#)'s function in any domain for which an ontology exists. A table of recommended ontology terms for [role](#) is given in [Table 4](#).

It is RECOMMENDED that these [role](#) property [URI](#)s identify terms that are compatible with the [type](#) properties of the [Feature](#)'s parent [Component](#). For example, a [role](#) of a [Feature](#) which belongs to a [Component](#) of type DNA might refer to terms from the Sequence Ontology. Likewise, for any feature that is a [SubComponent](#), the [role](#) SHOULD be compatible with the [type](#) of the [Component](#) that it links to through its `instanceOf` property.

The orientation property

The [orientation](#) property is OPTIONAL and has a data type of [URI](#). This can be used to indicate how any associated double-stranded [Feature](#) is oriented on the [elements](#) of a [Sequence](#) from their parent [Component](#). [Table 5](#) provides a list of REQUIRED [orientation](#) [URI](#)s. If a [Feature](#) object has an [orientation](#), then it MUST come from [Table 5](#).

6.4.1.1 SubComponent

The [SubComponent](#) class is a subclass of the [Feature](#) class that can be used to specify structural hierarchy. For example, the [Component](#) of a gene might contain four [SubComponent](#) objects: a promoter, RBS, CDS, and terminator, each linked to a [Component](#) that provides the complete definition. In turn, the [Component](#) of the promoter [SubComponent](#) might itself contain [SubComponent](#) objects defining various operator sites, etc.

Orientation URI	Description
http://sbols.org/v2#inline	The region specified by this Feature or Location is on the elements of a Sequence .
http://sbols.org/v2#reverseComplement	The region specified by this Feature or Location is on the reverse-complement mapping of the elements of a Sequence . The exact nature of this mapping depends on the encoding of the Sequence .

Table 5: REQUIRED URIs for the [orientation](#) property***The roleIntegration property***

A [roleIntegration](#) specifies the relationship between a [SubComponent](#) instance's own set of [role](#) properties and the set of [role](#) properties on the included [Component](#).

The [roleIntegration](#) property has a data type of [URI](#). A [SubComponent](#) instance with zero [role](#) properties MAY OPTIONALLY specify a [roleIntegration](#). A [SubComponent](#) instance with one or more [role](#) properties MUST specify a [roleIntegration](#) from Table 6. If zero [SubComponent](#) [role](#) properties are given and no [SubComponent](#) [roleIntegration](#) is given, then <http://sbols.org/v2#mergeRoles> is assumed. It is RECOMMENDED to specify [SubComponent](#) [role](#) values only if the result would differ from the [role](#) values belonging to this [SubComponent](#)'s included [Component](#).

roleIntegration URI	Description
http://sbols.org/v2#overrideRoles	In the context of this SubComponent , ignore any role given for the included Component . Instead use only the set of zero or more role properties given for this SubComponent .
http://sbols.org/v2#mergeRoles	Use the union of the two sets: both the set of zero or more role properties given for this SubComponent as well as the set of zero or more role properties given for the included Component .

Table 6: Each [roleIntegration](#) mode is associated with a rule governing how a [SubComponent](#)'s [role](#) values are to be combined with the included [Component](#)'s [role](#) values.***The instanceOf property***

The [instanceOf](#) property is a REQUIRED [URI](#) that refers to the [Component](#) providing the definition for this [SubComponent](#). Among other things, as described in the previous section, this [Component](#) effectively provides information about the [type](#) and [role](#) of the [SubComponent](#).

The [instanceOf](#) property MUST NOT refer to the same [Component](#) as the one that contains the [SubComponent](#). Furthermore, [SubComponent](#) objects MUST NOT form a cyclical chain of references via their [instanceOf](#) properties and the [Component](#) objects that contain them. For example, consider the [SubComponent](#) objects *A* and *B* and the [Component](#) objects *X* and *Y*. The reference chain “*X* has feature *A*, *A* is an instance of *Y*, *Y* has feature *B*, and *B* is an instance of *X*” is cyclical.

The hasLocation property

A [SubComponent](#) MAY have any number of [hasLocation](#) properties, each of type [URI](#), that MUST refer to [Location](#) objects that indicates the location of the [Sequence](#) from the [instanceOf](#) [Component](#) in a [Sequence](#) of the parent [Component](#).

If any [hasLocation](#) is defined, then there MUST BE precisely one [Sequence](#) in the [instanceOf](#) [Component](#), as otherwise this relationship is ill-defined.

If no `hasLocation` is defined, this indicates a part / sub-part relationship for which sequence details have not (yet) been determined or involving types for which sequence relationships are not relevant (e.g., inclusion of a reaction chain within a larger metabolic network).

Allowing multiple `Location` objects on a single `SubComponent` is intended to enable representation of discontinuous regions (for example, a coding sequence encoded across a set of exons with interspersed introns). As such, the `Location` objects of a single `SubComponent` MUST NOT specify overlapping regions, since it is not clear what this would mean. There is no such concern with different objects, however, which can freely overlap in `Location` (for example, specifying overlapping linkers for sequence assembly).

The sourceLocation property

The `sourceLocation` property allows for only a portion of a `Component`'s `Sequence` to be included, rather than its entirety. For example, when composing parts with certain assembly methods, some bases on the boundary may be removed or replaced. Another example is describing a deletion or replacement of a portion of a sequence.

A `SubComponent` MAY have any number of `sourceLocation` properties, each of type `URI`, that MUST refer to `Location` objects that indicate which `elements` of the `instanceOf Component`'s `Sequence` are used in defining the parent of the `SubComponent`.

If there are no `sourceLocation` properties, then the whole `Sequence` is assumed to be included.

6.4.1.2 ComponentReference

The `ComponentReference` class is a subclass of `Feature` that can be used to reference `Features` within `SubComponents`.

The inChildOf property

The `inChildOf` property is a REQUIRED `URI` that refers to a `SubComponent`. The `inChildOf` property MUST refer to a `SubComponent` pointed directly to by the parent of the `ComponentReference`. Specifically:

- If the parent of the `ComponentReference` is a `Component`, then `inChildOf` MUST be one of its `SubComponents`.
- If the parent of the `ComponentReference` is another `ComponentReference`, then `inChildOf` MUST be a `SubComponent` of the `Component` linked as `instanceOf` the parent's `inChildOf SubComponent`.

The hasFeature property

The `hasFeature` property is a REQUIRED `URI` that refers to a `Feature`.

This can be used to either link to the `Feature` being referenced or to chain hierarchically through additional layers of `SubComponent`.

- If the `Feature` is a `ComponentReference`, then that `ComponentReference` acts as a hierarchical link in a chain of references, and MUST be either a child of the `ComponentReference` linking to it via `hasFeature` or a child of the `Component` linked as `instanceOf` the `ComponentReference`'s `inChildOf SubComponent`.
- Otherwise, if the `hasFeature` refers to any other type of `Feature`, that `Feature` MUST be a child of the `Component` linked as `instanceOf` the `ComponentReference`'s `inChildOf SubComponent`.

For example, `ComponentReference` R1 looking into a `SubComponent` for a plasmid might link with `hasFeature` to its own child `ComponentReference` R2, which in turn looks within the `Component` defining the plasmid to the plasmid's CDS `SubComponent`, in turn using `hasFeature` to reference a `SequenceFeature` within the `Component` that defines that CDS.

6.4.1.3 LocalSubComponent

The [LocalSubComponent](#) class is a subclass of [Feature](#). This class serves as a way to create a placeholder in more complex [Components](#), such as a variable to be filled in later or a composite that exists only within the context of the parent [Component](#).

The hasLocation property

A [LocalSubComponent](#) MAY have any number of [hasLocation](#) properties, each of type [URI](#), that MUST refer to [Location](#) objects. These follow the same restrictions as for the [hasLocation](#) of a [SubComponent](#), notably that the [Locations](#) of [hasLocation](#) properties attached to the same [LocalSubComponent](#) MUST NOT overlap.

The type property

The [type](#) property is REQUIRED and contains one or more [URIs](#). The [type](#) property is identical to its use in [Component](#).

6.4.1.4 ExternallyDefined

The [ExternallyDefined](#) class has been introduced so that external definitions in databases like ChEBI or UniProt can be referenced.

The type property

The [type](#) property is REQUIRED and contains one or more [URIs](#). The [type](#) property is identical to its use in [Component](#).

The definition property

The [definition](#) property is REQUIRED and is of type [URI](#) that links to a canonical definition external to SBOL. When possible, such definitions SHOULD use the recommended external resources in [Section 7.6](#). For example, an [ExternallyDefined](#) simple chemical might link to ChEBI and a protein might link to UniProt.

6.4.1.5 SequenceFeature

The [SequenceFeature](#) class describes one or more regions of interest on the [Sequence](#) objects referred to by its parent [Component](#).

The hasLocation property

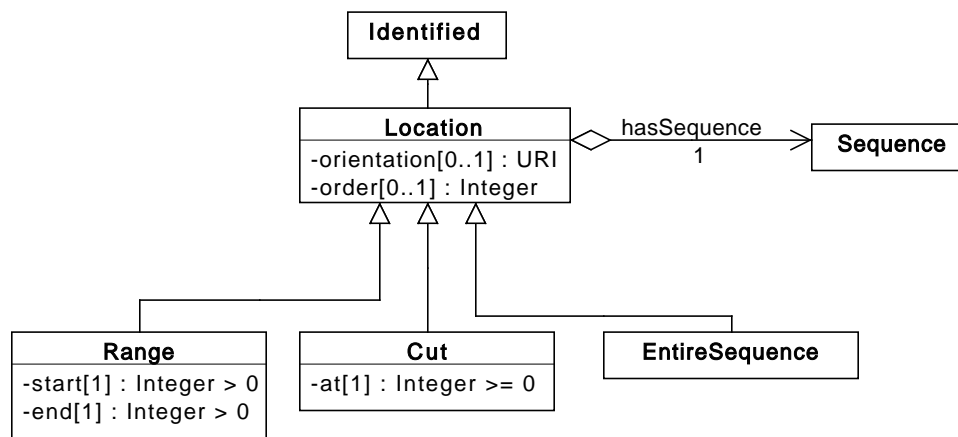
A [SequenceFeature](#) MAY have any number of [hasLocation](#) properties, each of type [URI](#), that MUST refer to [Location](#) objects. These follow the same restrictions as for the [hasLocation](#) of a [SubComponent](#), notably that the [Locations](#) of [hasLocation](#) properties attached to the same [SequenceFeature](#) MUST NOT overlap.

6.4.2 Location

The [Location](#) class (as shown in [Figure 10](#)) is used to represent the location of [Features](#) within [Sequences](#). This class is extended by the [Range](#), [Cut](#), and [EntireSequence](#) classes

The orientation property

The [orientation](#) property is OPTIONAL and has a data type of [URI](#). All subclasses of [Location](#) share this property, which can be used to indicate how any associated double-stranded [Feature](#) is oriented on the [elements](#) of a [Sequence](#) from their parent [Component](#). [Table 5](#) provides a list of REQUIRED [orientation](#) URIs. If a [Location](#) object has an [orientation](#), then it MUST come from [Table 5](#).

Figure 10: Diagram of the **Location** class and its associated properties.**The order property**

The **order** property is OPTIONAL and has a data type of **Integer**. If there are multiple **Location** objects associated with a **Feature**, the **order** property is used to specify the order (in increasing value) in which the specified **Locations** are to be joined to form the sequence of the **Feature**. Note that order values MAY be non-sequential and non-positive, if desired.

The hasSequence property

The **hasSequence** property is REQUIRED and MUST contain the **URI** of a **Sequence** object. All subclasses of **Location** share this property, which indicates which **Sequence** object referenced by the containing **Component** is referenced by the **Location**.

6.4.2.1 Range

A **Range** object specifies a region via discrete, inclusive **start** and **end** positions that correspond to indices for characters in the **elements String** of a **Sequence**.

Note that the index of the first location is 1, as is typical practice in biology, rather than 0, as is typical practice in computer science.

The start property

The **start** property specifies the inclusive starting position of the **Range**. This property is REQUIRED and MUST contain an **Integer** value greater than zero.

The end property

The **end** property specifies the inclusive ending position of the **Range**. This property is REQUIRED and MUST contain an **Integer** value greater than zero. In addition, this **Integer** value MUST be greater than or equal to that of the **start** property.

6.4.2.2 Cut

The **Cut** class has been introduced to enable the specification of a region between two discrete positions. This specification is accomplished using the **at** property, which specifies a discrete position that corresponds to the index of a character in the **elements String** of a **Sequence** (except in the case when **at** is equal to zero—see below).

The *at* property

The *at* property is REQUIRED and MUST contain an *Integer* value greater than or equal to zero. The region specified by the *Cut* is between the position specified by this property and the position that immediately follows it. When the *at* property is equal to zero, the specified region is immediately before the first discrete position or character in the *elements String* of a *Sequence*.

6.4.2.3 EntireSequence

The *EntireSequence* class does not have any additional properties. Use of this class indicates that the linked Sequence describes the entirety of the *Component* or *Feature* parent of this Location object.

6.4.3 Constraint

The *Constraint* class can be used to assert restrictions on the relationships of pairs of *Feature* objects contained by the same parent *Component*. Uses of this class include expressing containment (e.g., a plasmid transformed into a chassis strain), identity mappings (e.g., replacing a placeholder value with a complete definition), and expressing relative, sequence-based positions (e.g., the ordering of features within a template). Each *Constraint* includes the *subject*, *object*, and *restriction* properties.

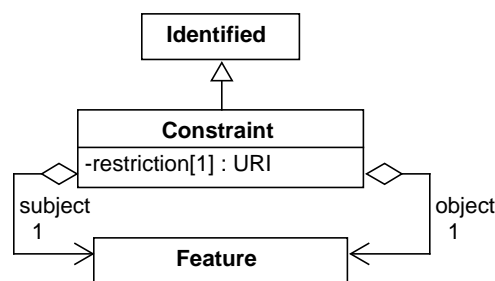


Figure 11: Diagram of the *Constraint* class and its associated properties.

The *subject* property

The *subject* property is REQUIRED and MUST contain a *URI* that refers to a *Feature* contained by the same parent *Component* that contains the *Constraint*.

The *object* property

The *object* property is REQUIRED and MUST contain a *URI* that refers to a *Feature* contained by the same parent *Component* that contains the *Constraint*. This *Feature* MUST NOT be the same *Feature* that the *Constraint* refers to via its *subject* property.

The *restriction* property

The *restriction* property is REQUIRED and has a data type of *URI*. This property MUST indicate the type of restriction on the locations, orientations, or identities of the *subject* and *object Feature* objects in relation to each other. The *URI* value of this property SHOULD come from the RECOMMENDED *URIs* in Table 7, Table 8, and Table 9.

Restriction URI	Description
http://sbols.org/v3#verifyIdentical	The subject and object , after tracing through any layers of ComponentReference , MUST both refer to SubComponent objects with the same instanceOf value or both refer to ExternallyDefined objects with the same definition . <i>Example: a promoter included via two different subsystems must be the identical.</i>
http://sbols.org/v3#differentFrom	The subject and object , after tracing through any layers of ComponentReference , MUST NOT both refer to SubComponent objects with the same instanceOf value or both refer to ExternallyDefined objects with the same definition . <i>Example: two fluorescent reporters must be different.</i>
http://sbols.org/v3#replaces	In the context of the parent object of the Constraint , information about the subject should be used in place of all instances of the object . <i>Example: the J23101 promoter replaces a generic promoter.</i>
http://sbols.org/v3#sameOrientationAs	The subject and object Component objects MUST have the same orientation. <i>Example: a promoter has the same orientation as the coding sequence it controls.</i>
http://sbols.org/v2#oppositeOrientationAs	The subject and object Component objects MUST have opposite orientations. <i>Example: a promoter has the opposite orientation as an invertase-activated coding sequence it controls.</i>

Table 7: RECOMMENDED URIs for expressing identity and orientation with the **restriction** property.

Restriction URI	Description
http://sbols.org/v3#isDisjointFrom	The subject and object do not overlap in space. <i>Example: a plasmid is disjoint from a chromosome.</i>
http://sbols.org/v3#strictlyContains	The subject entirely contains the object : they do not share a boundary. <i>Example: a cell contains a plasmid</i>
http://sbols.org/v3#contains	The subject contains the object and they might or might not share a boundary (i.e., union of strictlyContains , equals , and covers). <i>Example: a cell contains a protein that may or may not bind to its membrane.</i>
http://sbols.org/v3#equals	The subject and object occupy the same location in space. <i>Example: a small molecule is distributed throughout an entire sample.</i>
http://sbols.org/v3#meets	The subject and object are connected at a shared boundary. <i>Example: two strains of adherent cells meet at their membranes.</i>
http://sbols.org/v3#covers	The subject contains the object but also shares a boundary. <i>Example: a cell covers its transmembrane proteins.</i>
http://sbols.org/v3#overlaps	The subject and object overlap in space, but portions of each are outside of the other. <i>Example: a transmembrane protein overlaps the cell membrane.</i>

Table 8: RECOMMENDED URIs for expressing topological relations with the **restriction** property.

6.4.4 Interaction

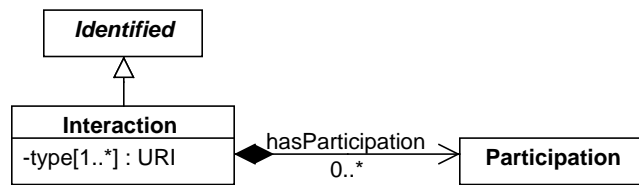
The **Interaction** class (as shown in Figure 12) provides more detailed description of how the **Feature** objects of a **Component** are intended to work together. For example, this class can be used to represent different forms of genetic regulation (e.g., transcriptional activation or repression), processes from the central dogma of biology (e.g. transcription and translation), and other basic molecular interactions (e.g., non-covalent binding or enzymatic phosphorylation). Each **Interaction** includes **type** properties that refer to descriptive ontology terms and **hasParticipation** properties that describe which **Feature** objects participate in which ways in the **Interaction**.

Restriction URI	Description	
http://sbols.org/v3#precedes	The start of the location for subject is less than the start of the location for object (i.e., union of strictlyPrecedes , meets , and overlaps). <i>Example: a promoter precedes a ribosome entry site, but the exact boundary between the two will be determined by sequence optimization and assembly planning.</i>	15
http://sbols.org/v3#strictlyPrecedes	The end of the location for subject is less than the start of the location for object . <i>Example: a promoter strictly precedes a terminator (with a CDS between them).</i>	16
http://sbols.org/v3#meets	The end of the location for subject is equal to the start of the location for object . Note: this is a stronger interpretation of meets from Table 8 in the context of a linear sequence. <i>Example: the 3' region adjacent to a blunt restriction site meets the 5' region adjacent to the site.</i>	17
http://sbols.org/v3#overlaps	The start of the location for subject is before the start of the location for object and the end of the location for subject is before the end of the location for object . Note: this is a stronger interpretation of overlaps from Table 8 in the context of a linear sequence. <i>Example: two adjacent oligos overlap in a Gibson assembly plan.</i>	18
http://sbols.org/v3#contains	The start of the location for subject is less than or equal to the start of the location for object and the end of the location for subject is greater than or equal to the end of the location for object (i.e., union of strictlyContains , equals , finishes , and starts). Note: this is a stronger interpretation of contains from Table 8 in the context of a linear sequence. <i>Example: a composite part contains a promoter.</i>	19
http://sbols.org/v3#strictlyContains	The start of the location for subject is before the start of the location for object and the end of the location for subject is after the end of the location for object . Note: this is a stronger interpretation of strictlyContains from Table 8 in the context of a linear sequence. <i>Example: an RNA transcript strictly contains an intron.</i>	20
http://sbols.org/v3#equals	The start and end of the location for subject are equal to the start and end of the location for object . Note: this is a stronger interpretation of equals from Table 8 in the context of a linear sequence. <i>Example: the transcribed region of a CDS part equals the entire part.</i>	21
http://sbols.org/v3#finishes	The start of the location for subject is after the start of the location for object and the end of the location for subject is equal to the end of the location for object . <i>Example: a terminator finishes an expression cassette.</i>	22
http://sbols.org/v3#starts	The start of the location for subject is equal to the start of the location for object and the end of the location for subject is before the end of the location for object . <i>Example: a promoter starts an expression cassette.</i>	23

Table 9: RECOMMENDED URIs for expressing sequential relations with the **restriction** property.**The type property**

An **Interaction** is REQUIRED to have one or more **type** properties, each of type **URI**, that describes the behavior represented by an **Interaction**.

Each **type** property MUST identify terms from appropriate ontologies. It is RECOMMENDED that exactly one **URI** specified by a **type** property refer to a term from the occurring entity branch of the **Systems Biology Ontology (SBO)**. Table 10 provides a partial list of possible SBO terms for the **type** property and their corresponding URIs.

Figure 12: Diagram of the [Interaction](#) class and its associated properties.

Interaction Type	URI for SBO Term
Inhibition	http://identifiers.org/biomodels.sbo/SBO:0000169
Stimulation	http://identifiers.org/biomodels.sbo/SBO:0000170
Biochemical Reaction	http://identifiers.org/biomodels.sbo/SBO:0000176
Non-Covalent Binding	http://identifiers.org/biomodels.sbo/SBO:0000177
Degradation	http://identifiers.org/biomodels.sbo/SBO:0000179
Genetic Production	http://identifiers.org/biomodels.sbo/SBO:0000589
Control	http://identifiers.org/biomodels.sbo/SBO:0000168

Table 10: Partial list of SBO terms to specify the [type](#) property of an [Interaction](#).

If an [Interaction](#) is well described by one of the terms from [Table 10](#), then a [type](#) property MUST refer to the [URI](#) that identifies this term. Lastly, if there are multiple [type](#) properties for an [Interaction](#), then they MUST identify non-conflicting terms. For example, the SBO terms “stimulation” and “inhibition” would conflict.

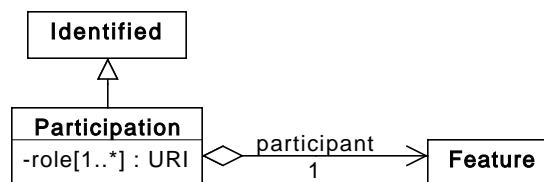
The hasParticipation property

An [Interaction](#) MAY have any number of [hasParticipation](#) properties, each of type [URI](#), that MUST reference a [Participation](#) object, each of which identifies the [role](#) that its referenced [Feature](#) plays in the [Interaction](#).

Even though an [Interaction](#) generally contains at least one [Participation](#), the case of zero [Participation](#) objects is allowed because it is plausible that a designer might want to specify that an [Interaction](#) will exist, even if its [participants](#) have not yet been determined.

6.4.4.1 Participation

Each [Participation](#) (see [Figure 13](#)) represents how a particular [Feature](#) behaves in its parent [Interaction](#).

Figure 13: Diagram of the [Participation](#) class and its associated properties.

The role property

A **Participation** is REQUIRED to have one or more **role** properties, each of type **URI**, that describes the behavior of a **Participation** (and by extension its referenced **Feature**) in the context of its parent **Interaction**.

Each **role** property MUST identify terms from appropriate ontologies. It is RECOMMENDED that exactly one **URI** specified by a **role** property refer to a term from the participant role branch of the SBO. Table 11 provides a partial list of possible SBO terms for the **role** properties and their corresponding **URIs**.

Participation Role	URI for SBO Term	Interaction Types
Inhibitor	http://identifiers.org/biomodels.sbo/SBO:0000020	Inhibition
Inhibited	http://identifiers.org/biomodels.sbo/SBO:0000642	Inhibition
Stimulator	http://identifiers.org/biomodels.sbo/SBO:0000459	Stimulation
Stimulated	http://identifiers.org/biomodels.sbo/SBO:0000643	Stimulation
Reactant	http://identifiers.org/biomodels.sbo/SBO:0000010	Non-Covalent Binding, Degradation Biochemical Reaction
Product	http://identifiers.org/biomodels.sbo/SBO:0000011	Non-Covalent Binding, Genetic Production, Biochemical Reaction
Promoter	http://identifiers.org/biomodels.sbo/SBO:0000598	Inhibition, Stimulation, Genetic Production
Modifier	http://identifiers.org/biomodels.sbo/SBO:0000019	Biochemical Reaction, Control
Modified	http://identifiers.org/biomodels.sbo/SBO:0000644	Biochemical Reaction, Control
Template	http://identifiers.org/biomodels.sbo/SBO:0000645	Genetic Production

Table 11: Partial list of SBO terms to specify the **role** properties of a **Participation**.

If a **Participation** is well described by one of the terms from Table 11, then a **role** property MUST refer to the **URI** that identifies this term. Also, if a **Participation** belongs to an **Interaction** that has a type listed in Table 10, then the **Participation** SHOULD have a role that is cross-listed with this type in Table 11. Lastly, if there are multiple **role** properties for a **Participation**, then they MUST identify non-conflicting terms. For example, the SBO terms “stimulator” and “inhibitor” would conflict.

The participant property

The **participant** property MUST specify precisely one **Feature** object that plays the designated role in its parent **Interaction** object.

6.4.5 Interface

The **Interface** class (shown in Figure 14) is a way of explicitly specifying the interface of a **Component**.

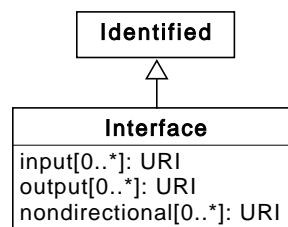


Figure 14: Diagram of the **Interface** class and its associated properties.

The input property

An **Interface** MAY have any number of **input** properties, each of type **URI**, that MUST reference a **Feature** object in the same **Component**.

The output property

An **Interface** MAY have any number of **output** properties, each of type **URI**, that MUST reference a **Feature** object in the same **Component**.

The nondirectional property

An **Interface** MAY have any number of **nondirectional** properties, each of type **URI**, that MUST reference a **Feature** object in the same **Component**. Note that nondirectional can imply both bidirectional as well as situations where there are no flows (for instance – a physical interface).

6.5 CombinatorialDerivation

The purpose of the **CombinatorialDerivation** class is to specify combinatorial biological designs without having to specify every possible design variant. For example, a **CombinatorialDerivation** can be used to specify a library of reporter gene variants that include different promoters and RBSs without having to specify a **Component** for every possible combination of promoter, RBS, and CDS in the library. **Component** objects that realize a **CombinatorialDerivation** can be derived in accordance with the class properties **template**, **hasVariableComponent**, and **strategy** (see Figure 15).

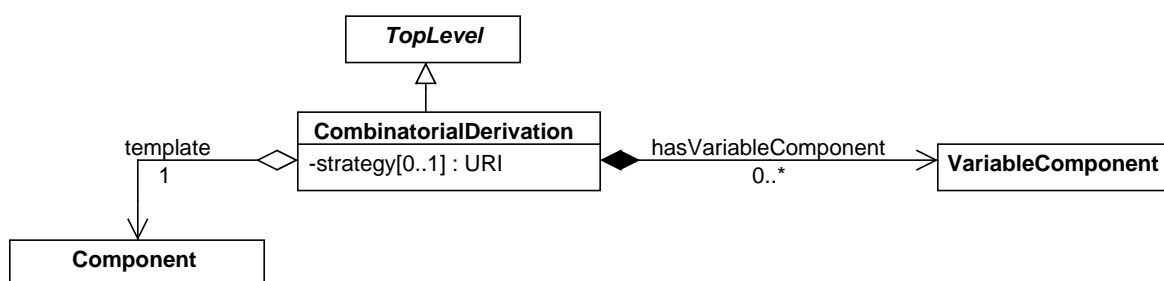


Figure 15: Diagram of the **CombinatorialDerivation** class and its associated properties.

The template property

The **template** property is REQUIRED and MUST contain a URI that refers to a **Component**. This **Component** is expected to serve as a template for the derivation of new **Component** objects. Consequently, its **hasFeature** properties SHOULD contain one or more **SubComponent** objects that describe its substructure (referred to hereafter as template **SubComponent** objects), and its **hasConstraint** property MAY also contain one or more **Constraint** objects that constrain this substructure.

When a **Component** is derived in accordance with a **CombinatorialDerivation**, the **prov:wasDerivedFrom** property of the derived **Component** SHOULD refer to the **CombinatorialDerivation**. When multiple **Component** objects are derived in accordance with the same **CombinatorialDerivation**, they MAY be referred to by the **member** property of a **Collection**, in which case the **prov:wasDerivedFrom** property of the **Collection** SHOULD also refer to this **CombinatorialDerivation**.

If the **type** property of the template **Component** contains one or more URIs, then the **type** property of any derived **Component** SHOULD also contain those URIs. The same holds true for the **role** properties of these **Component**

objects.

The *hasVariableComponent* property

Each **VariableComponent** child of a **CombinatorialDerivation** defines the set of possible values for one of the variables in the **template**. A **CombinatorialDerivation** object can have zero or more **hasVariableComponent** properties, each of type **URI**, specifying a **VariableComponent**. The set of **hasVariableComponent** properties MUST NOT contain two or more **VariableComponent** objects that refer to the same template **SubComponent** via their **variable** properties (i.e., do not define the same variable twice).

The **variable** properties of **VariableComponent** objects control which **SubComponent** objects in the **template** are modified in a derived **Component**. If no **variable** property of one of these **VariableComponent** objects refers to a template **SubComponent**, then it is not a variable and the derived object SHOULD have a **SubComponent** with identical **instanceOf** and **sourceLocation** properties and a **prov:wasDerivedFrom** property that refers to the template **SubComponent**.

If a **SubComponent** in the **template** is referred to by some **variable** in a **VariableComponent**, then it is a variable and it SHOULD be replaced in the derived **Component** by a number of **SubComponent** objects constrained by the number specified by the **cardinality** property of the **VariableComponent** (see Table 13). Each **instanceOf** property of such a **SubComponent** object in the derived **Component** MUST refer to a **Component** object specified by a **variant**, contained within a **variantCollection**, or derived from a **variantDerivation** of the **VariableComponent**.

Finally, all derived **SubComponent** objects MUST follow the **restriction** properties of any **Constraint** objects that refer to their corresponding template **SubComponent**, and SHOULD have values of **role** that contain the same values as the **role** in the template **SubComponent**.

The *strategy* property

The **strategy** property is OPTIONAL and has a data type of **URI**. Table 12 provides a list of REQUIRED **strategy** URIs. If the **strategy** property is not empty, then it MUST contain a URI from Table 12. This property recommends how many **Component** objects SHOULD be derived from the template **Component**.

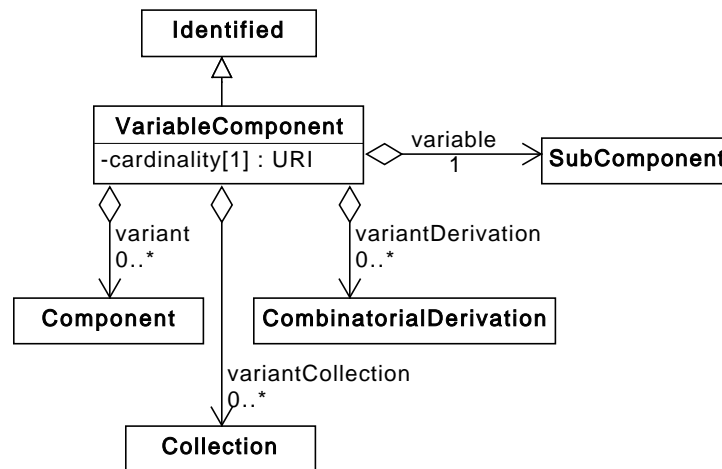
Strategy URI	Description
http://sbols.org/v2#enumerate	Derivation SHOULD produce all possible Component objects specified by the CombinatorialDerivation .
http://sbols.org/v2#sample	Derivation SHOULD produce a subset of possible Component objects specified by CombinatorialDerivation . The manner in which this subset is chosen is left unspecified.

Table 12: REQUIRED URIs for the **strategy** property.

6.5.1 VariableComponent

As described above, the **VariableComponent** class specifies a variable and set of values that will replace one of the **SubComponent** objects in the **template** of a **CombinatorialDerivation**. The variable is specified by the **variable** property, and the set of values is defined by the union of **Component** objects referred to by the **variant**, **variantCollection**, and **variantDerivation** properties.

Note that this union is intended to be a set and not a multi-set. For example, if the **variant** property contains a **Component** *A* and the **variantCollection** property has a **Collection** containing both **Component** *A* and **Component** *B*, then *A* SHOULD NOT be selected twice during enumeration, and it SHOULD NOT be selected twice as much as *B* during sampling.

Figure 16: Diagram of the **VariableComponent** class and its associated properties.**The variable property**

The **variable** property is REQUIRED and MUST contain a URI that refers to a template **SubComponent** in the **template Component** referred to by this **VariableComponent**'s parent **CombinatorialDerivation**

The variant property

A **VariableComponent** object can have zero or more **variant** properties, each of type **URI**, specifying a **Component** object. This property specifies individual **Component** objects to serve as options when deriving a new **SubComponent** for the **variable SubComponent** from the **template**.

The variantCollection property

A **VariableComponent** object can have zero or more **variantCollection** properties, each of type **URI**, specifying a **Collection** object. Such a **Collection** MUST NOT contain any objects besides **Component** objects or **Collection** objects that themselves contain only **Component** or **Collection** objects. This property enables the specification of existing groups of **Component** objects to serve as options.

The variantDerivation property

A **VariableComponent** object can have zero or more **variantDerivation** properties, each of type **URI**, specifying a **CombinatorialDerivation** object. This property enables the specification of **Component** objects derived in accordance with another **CombinatorialDerivation** to serve as options when deriving a new **SubComponent** for the **variable SubComponent** from the **template**. The **variantDerivation** properties of a **VariableComponent** MUST NOT refer to the **CombinatorialDerivation** that contains this **VariableComponent**. Furthermore, such **VariableComponent** objects MUST NOT form a cyclical chain of references via their **variantDerivation** properties and the **CombinatorialDerivation** objects that contain them.

The cardinality property

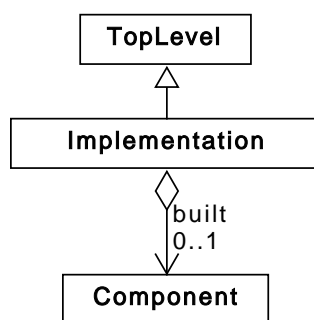
The **cardinality** property is REQUIRED and has type of **URI**. This property specifies how many **SubComponent** objects SHOULD be derived from the template **SubComponent** during the derivation of a new **Component**. The **URI** value of this property MUST come from the URIs provided in **Table 13**.

Cardinality URI	Description
http://sbols.org/v2#zeroOrOne	No more than one SubComponent in the derived Component SHOULD have a prov:wasDerivedFrom property that refers to the template SubComponent .
http://sbols.org/v2#one	Exactly one SubComponent in the derived Component SHOULD have a prov:wasDerivedFrom property that refers to the template SubComponent .
http://sbols.org/v2#zeroOrMore	Any number of SubComponent objects in the derived Component MAY have prov:wasDerivedFrom properties that refer to the template SubComponent .
http://sbols.org/v2#oneOrMore	At least one SubComponent in the derived Component SHOULD have a prov:wasDerivedFrom property that refers to the template SubComponent .

Table 13: REQUIRED URIs for the [cardinality](#) property.

6.6 Implementation

An [Implementation](#) represents a realized instance of a [Component](#), such a sample of DNA resulting from fabricating a genetic design or an aliquot of a specified reagent. Importantly, an [Implementation](#) can be associated with a laboratory sample that was already built, or that is planned to be built in the future. An [Implementation](#) can also represent virtual and simulated instances. An [Implementation](#) may be linked back to its original design using the [prov:wasDerivedFrom](#) property inherited from the [Identified](#) superclass. An [Implementation](#) may also link to a [Component](#) that specifies its realized structure and/or function.

Figure 17: Diagram of the [Implementation](#) class and its associated properties.

The *built* property

The [built](#) property is OPTIONAL and MAY contain a URI that MUST refer to a [Component](#). This [Component](#) is intended to describe the actual physical structure and/or functional behavior of the [Implementation](#). When the built property refers to a [Component](#) that is also linked to the [Implementation](#) via PROV-O properties such as [prov:wasDerivedFrom](#) (see [Section A.1](#)), it can be inferred that the actual structure and/or function of the [Implementation](#) matches its original design. When the [built](#) property refers to a different [Component](#), it can be inferred that the [Implementation](#) has deviated from the original design. For example, the latter could be used to document when the DNA sequencing results for an assembled construct do not match the original target sequence.

6.7 ExperimentalData

The purpose of the [ExperimentalData](#) class is to aggregate links to experimental data files. An [ExperimentalData](#) is typically associated with a single sample, lab instrument, or experimental condition and can be used to describe the output of the test phase of a design-build-test-learn workflow. For an example of the latter, see [Figure 28](#).

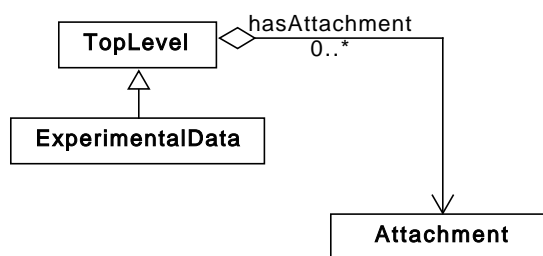


Figure 18: Diagram of the [ExperimentalData](#) class and its associated properties.

As shown in [Figure 18](#), the [ExperimentalData](#) class aggregates links to experimental data files using the OPTIONAL [hasAttachment](#) property that it inherits from the [TopLevel](#) class.

6.8 Model

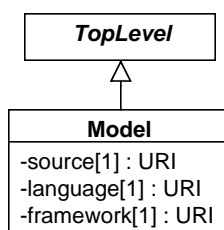


Figure 19: Diagram of the [Model](#) class and its associated properties.

The purpose of the [Model](#) class is to serve as a placeholder for an external computational model and provide additional meta-data to enable better reasoning about the contents of this model. In this way, there is minimal duplication of standardization efforts and users of SBOL can elaborate descriptions of [Component](#) function in the language of their choice.

The meta-data provided by the [Model](#) class include the following properties: the [source](#) or location of the actual content of the model, the [language](#) in which the model is implemented, and the model's [framework](#).

The source property

The [source](#) property is REQUIRED and MUST contain a [URI](#) reference to the source file for a model.

The language property

The [language](#) property is REQUIRED and MUST contain a [URI](#) that specifies the language in which the model is implemented. It is RECOMMENDED that this [URI](#) refer to a term from the EMBRACE Data and Methods (EDAM) ontology. [Table 14](#) provides a list of a few suggested languages from this ontology and their [URIs](#). If the [language](#) property of a [Model](#) is well-described by one these terms, then it MUST contain the [URI](#) for this term as its value.

The framework property

The [framework](#) property is REQUIRED and MUST contain a [URI](#) that specifies the framework in which the model is implemented. It is RECOMMENDED this [URI](#) refer to a term from the modeling framework branch of the SBO when possible. A few suggested modeling frameworks and their corresponding [URIs](#) are shown in [Table 15](#). If the

Model Language	URI for EDAM Term
SBML	http://identifiers.org/edam/format_2585
CellML	http://identifiers.org/edam/format_3240
BioPAX	http://identifiers.org/edam/format_3156

Table 14: Terms from the EDAM ontology to specify the [language](#) property of a [Model](#).

[framework](#) property of a [Model](#) is well-described by one these terms, then it MUST contain the [URI](#) for this term as its value.

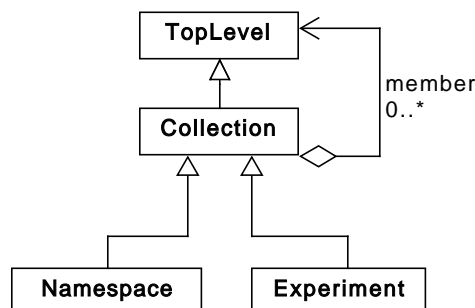
Framework	URI for SBO Term
Continuous	http://identifiers.org/biomodels.sbo/SBO:0000062
Discrete	http://identifiers.org/biomodels.sbo/SBO:0000063

Table 15: SBO terms to specify the [framework](#) property of a [Model](#).

6.9 Collection

The [Collection](#) class is a class that groups together a set of [TopLevel](#) objects that have something in common. Some examples of [Collection](#) objects:

- Results of a query to find all [Component](#) objects in a repository that function as promoters.
- A set of [Component](#) objects representing a library of genetic logic gates.
- A “parts list” for [Component](#) with a complex design, containing both that component and all of the [Component](#), [Sequence](#), and [Model](#) objects used to provide its full specification.

Figure 20: Diagram of the [Collection](#) class and its associated properties.

The *member* property

A [Collection](#) object can have zero or more [member](#) properties, each of type [URI](#) specifying a [TopLevel](#) object.

6.9.1 Namespace

The **Namespace** class is a subclass of **Collection** and is used to define **member** entities that share the same URI prefix. Namely, all linked objects MUST have a URI prefix matching the URI of the **Namespace** object.

6.9.2 Experiment

The purpose of the **Experiment** class is to aggregate **ExperimentalData** objects for subsequent analysis, usually in accordance with an experimental design. Namely, the **member** properties of an **Experiment** MUST refer to **ExperimentalData** objects.

6.10 Attachment

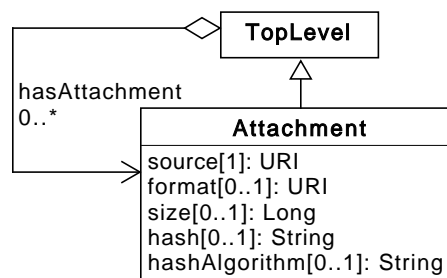


Figure 21: Diagram of the **Attachment** class and its associated properties.

The purpose of the **Attachment** class is to serve as a general container for data files, especially experimental data files. It provides a means for linking files and metadata to SBOL designs.

The meta-data provided by the **Attachment** class include the following properties: the **source** or location of the actual file of the attachment, the **format** of the file, the **size** of the file, and the **hash** for the file.

The source property

The **source** property is REQUIRED and MUST contain a **URI** reference to the source file.

The format property

The **format** property is OPTIONAL and MAY contain a **URI** that specifies the format of the attached file. It is RECOMMENDED that this **URI** refer to a term from the EMBRACE Data and Methods (EDAM) ontology.

The size property

The **size** property is OPTIONAL and MAY contain a long indicating the file size in bytes.

The hash property

The **hash** property is OPTIONAL and MAY contain a hash value for the file contents represented as a hexadecimal digest.

The hashAlgorithm property

The **hashAlgorithm** property is OPTIONAL and MAY contain the name of the hash algorithm used to generate the value of the **hash** property. The value of this property SHOULD be a hash name string from the **IANA Named Information Hash Algorithm Registry**, of which **sha3-256** is currently RECOMMENDED. If the **hash** property is set,

then `hashAlgorithm` MUST be set as well.

6.11 Annotation and Extension of SBOL

SBOL intentionally does not attempt to describe how all types of biological design data should be captured, since many of these data types (e.g., biological context and design performance metrics) are already covered by other standards, or lack a clear consensus on their proper representation, or are outside of the scope of SBOL.

SBOL is built upon the Resource Description Framework (RDF), and therefore can be used in conjunction with complementary standards as described in [Section A](#). For example, use of the PROV-O ontology is recommended to capture provenance (see [Section A.1](#)). Additionally, user-defined RDF can be used in conjunction with SBOL objects to capture custom application-specific information that does not yet have a standardized representation. This annotation and extension mechanism is designed to enable new types of data to be easily incorporated into the SBOL standard once there is community consensus on their proper representation.

Several methods are supported for connecting the SBOL data model with other types of application-specific data:

- Custom data can be added to an SBOL object by annotating that object with non-conflicting properties. These properties could contain `literal` data types such as `Strings` or `URIs` that require a resolution mechanism to obtain external data. An example is annotating a `Component` with a property that contains a `String` description and `URI` for the parts registry from which its source data was originally imported.
- Custom data in the form of independent objects can participate in the SBOL data model if they are assigned one of the SBOL types `Identified` or `TopLevel`. An example is an RDF object that is annotated such that it represents a data sheet that describes the performance of a `Component` in a particular context.
- Finally, just as custom objects can be embedded in an SBOL document, external documents can embed or refer to SBOL objects. Support for this last case is not explicitly provided in this specification. Rather, this case depends on the external non-SBOL system managing its relationship to SBOL and data serialized in RDF, and is included here for completeness.

Each `Identified` object MAY be annotated with application-specific properties, which MUST be labelled using RDF predicates outside of the SBOL namespace. Additionally, application-specific types may be used in conjunction with the SBOL data model. These application-specific types MUST have two `rdf:type` properties: one type outside of the SBOL namespace AND an additional SBOL type of either:

- `TopLevel`, if the object is to be considered an SBOL top level (i.e., not owned by another object)
- `Identified`, if the object is not to be considered an SBOL top level (i.e., is owned by another object)

As with SBOL `Identified` objects, custom `Identified` objects (and thus also custom `TopLevel` objects) MAY also include the properties `displayId`, `name`, `description`, etc.

7 Recommended Best Practices

7.1 SBOL Versions

To differentiate between major versions of SBOL, different namespaces are used. For example, SBOL3 has the namespace <http://sbols.org/v3#>, while SBOL2 has the namespace <http://sbols.org/v2#>. These different versions of SBOL SHOULD NOT be semantically mixed. For example, an SBOL 3.x [SubComponent](#) SHOULD NOT refer to an SBOL 2.x [ComponentInstance](#), and, likewise, an SBOL 2.x [ComponentInstance](#) SHOULD NOT refer to an SBOL 1.x [DnaComponent](#).

7.2 Compliant SBOL Objects

Maintaining unique URIs for all SBOL objects can be challenging. To reduce this burden, users of SBOL 3.x are encouraged to follow a few simple rules when constructing the URIs and related properties for SBOL objects. When these rules are followed in constructing an SBOL object, we say that this object is *compliant*. These rules are as follows:

Compliant URIs for [TopLevel](#) objects MUST conform to the following pattern:

`<namespace>/<collection_structure>/<displayName>`

The `<namespace>` token MAY further decompose into `<domain>/<root>` tokens. The `<root>` and `<collection_structure>` tokens may optionally be omitted; alternatively, they may consist of an arbitrary number of delimiter-separated layers. Note that this pattern means that SBOL-compliant URIs can be automatically decomposed with the aid of a [Namespace](#). SBOL-compliant objects can be easily remapped into new namespaces by changing only the `<namespace>`.

Consider, for example, the SBOL-compliant [URI](#):

`"https://synbiohub.org/igem/2017_distribution/promoters/constitutive/BBa_J23101"`

in [Namespace](#) `"https://synbiohub.org/igem/2017_distribution"`. This [URI](#) can be decomposed as follows:

namespace:	<code>"https://synbiohub.org/igem/2017_distribution"</code>
domain:	<code>"https://synbiohub.org"</code>
root:	<code>"igem/2017_distribution"</code>
collection:	<code>"promoters/constitutive"</code>
displayName:	<code>"BBa_J23101"</code>

SBOL-compliant URIs also facilitate auto-construction of child objects with unique URIs. Child objects of [TopLevel](#) objects with compliant URIs MUST conform to the following pattern:

`"<parent_uri>/<child_type><child_type_counter>"` where the `<parent_uri>` refers to the URI of the parent object, the `<child_type>` refers to the SBOL class of the child object, and `<child_type_counter>` is a unique index for the child object. The `<child_type_counter>` of a new object SHOULD be calculated at time of object creation as 1 + the maximum `<child_type_counter>` for each `<child_type>` object in the parent (e.g., `"<parent_uri>/SequenceAnnotation37"`). Note that numbering is independent for each type, so a [Component](#) can have children `"SubComponent37"` and `"Constraint37"`.

All examples in this specification use compliant URIs.

7.3 Versioning SBOL Objects

SBOL 3.x does not specify an explicit versioning scheme. Rather it is left for experimentation across different tools. This allows version information to be included in the root (e.g., GitHub style: “igem/HEAD/”), collection structure (e.g., “promoters/constitutive/2/”), in tool-specific conventions on `displayId` (e.g., “BBa_J23101_v2”) or in information outside of the [URI](#) (e.g., by attaching `prov:wasRevisionOf` properties).

7.4 Annotations: Embedded Objects vs. External References

When annotating an SBOL document with additional information, there are two general methods that can be used:

- Embed the information in the SBOL document using properties outside of the SBOL namespace.
- Store the information separately and annotate the SBOL document with [URIs](#) that point to it.

In theory, either method can be used in any case. (Note that a third case not discussed here is to annotate external objects with links to SBOL documents, rather than annotating SBOL documents with links to external objects.)

In practice, embedding large amounts of non-SBOL data into SBOL documents is likely to cause problems for people and software tools trying to manage and exchange such documents. Therefore, it is RECOMMENDED that small amounts of information (e.g., design notes or preferred graphical layout) be embedded in the SBOL model, while large amounts of information (e.g., the contents of the scientific publication from which a model was derived or flow cytometry data that characterizes performance) be linked with URIs pointing to external resources. The boundary between “small” and “large” is left deliberately vague, recognizing that it will likely depend on the particulars of a given SBOL application.

7.5 Completeness and Validation

RDF documents containing serialized SBOL objects might or might not be entirely self-contained. A SBOL document is self-contained or “complete” if every SBOL object referred to in the document is contained in the document. It is RECOMMENDED that serializations be complete whenever practical. In other words, when serializing an SBOL object, serialize all of the other objects that it points to, then serialize all of the other objects that these objects point to, etc., until the document is complete.

It is important to note that there is no guarantee that an RDF document contains valid SBOL. When SBOL objects are read from an RDF document, the program doing so SHOULD verify that all of the property values encoded therein have the correct data type (e.g., that the object pointed to by the `Sequence` property of a `Component` is really a `Sequence`). For complete files, this validation can be carried out entirely locally. For files that are not complete, an implementation either needs to have a means of validating those external references (e.g., by retrieving them from a repository), or it needs to mark them as unverified and not depend on their correctness.

7.6 Recommended Ontologies for External Terms

External ontologies and controlled vocabularies are an integral part of SBOL. SBOL uses [URIs](#) to access existing biological information through these resources. New SBOL-specific terms are defined only when necessary. For example, `Component` types, such as DNA or protein, are described using Systems Biology Ontology (SBO) terms. Similarly, the `roles` of a DNA or RNA `Component` are described via Sequence Ontology (SO) terms. Although RECOMMENDED ontologies have been indicated in relevant sections where possible, other resources providing similar terms can also be used. A summary of these external sources can be found in [Table 16](#).

The URIs for ontological terms SHOULD come from identifiers.org. However, it is acceptable to use terms from purl.org as an alternative, for example when RDF tooling requires URIs to be represented as compliant QNames. SBOL software may convert between these forms as required.

SBOL Entity	Property	Preferred External Resource	More Information
Component	type	SBO (physical entity branch)	http://www.ebi.ac.uk/sbo/main/
	type	SO (nucleic acid topology)	http://www.sequenceontology.org
	role	SO (<i>DNA</i> or <i>RNA</i>)	http://www.sequenceontology.org
	role	CHEBI (<i>small molecule</i>)	https://www.ebi.ac.uk/chebi/
	role	UniProt (<i>protein</i>)	https://www.uniprot.org/
	role	NCIT (<i>samples</i>)	https://ncithesaurus.nci.nih.gov/
Interaction	type	SBO (occurring entity branch)	http://www.ebi.ac.uk/sbo/main/
Participation	role	SBO (participant roles branch)	http://www.ebi.ac.uk/sbo/main/
Model	language	EDAM	http://bioportal.bioontology.org/ontologies/EDAM
om:Measure	framework	SBO (modeling framework branch)	http://www.ebi.ac.uk/sbo/main/
	type	SBO (systems description parameters)	http://www.ebi.ac.uk/sbo/main/

Table 16: Preferred external resources from which to draw values for various SBOL properties.

7.7 Annotating Entities with Date & Time

Entities in an SBOL document can be annotated with creation and modification dates. It is RECOMMENDED that predicates, or properties, from DCMI Metadata Terms SHOULD be used to include date and time information. The **created** and **modified** terms SHOULD respectively be used to annotate SBOL entities with creation and modification dates. Date and time values SHOULD be expressed using the XML Schema **DateTime** datatype (Biron et al., 2004). For example, “2016-03-16T20:12:00Z” specifies that the day is 16 March 2016 and the time is 20:12pm in UTC (Coordinated Universal Time).

7.8 Annotating Entities with Authorship information

Authorship information should ideally be added to **TopLevel** entities where possible. It is RECOMMENDED that the **creator** DCMI Metadata term SHOULD be used to annotate SBOL entities with authorship information using free text. This property can be repeated for each author.

7.9 Host Context / Ontologies for Experiments

7.9.1 Mixtures via Components

Any **Component** can be interpreted as specifying a mixture of the material entity (SBO:0000240) **Features** that it includes. The amount of each such instance included in the mixture SHOULD be specified by attaching a **om:Measure** with a **type** set to the appropriate SBO term. The SBO terms that are RECOMMENDED as appropriate are members of the Systems Description Parameter (SBO:0000545) branch of SBO. Examples include:

- SBO:0000540: fraction of an entity pool (e.g., 1/3 CHO cells, 2/3 HEK cells)
- SBO:0000472: molar concentration of an entity (e.g., 1 mM Arabinose)
- SBO:0000361: amount of an entity pool (e.g., 200 uL M9 media)

Mixtures MAY be defined recursively, as mixtures of mixtures of mixtures, etc.

7.9.2 Media, Inducers, and Other Reagents

Each reagent, whether “atomic” (e.g., rainbow bead control) or mixture (e.g., M9 media), SHOULD be represented as a **Component**.

The roles of reagents may vary in context: for example, Arabinose may serve as an inducer or as a media car-

bon source. As such, role SHOULD be indicated by an NCI Thesaurus (NCIT) term in a [role](#) property of the [SubComponent](#). Examples include:

- NCIT:C64356: Positive Control
- NCIT:C48694: Cell
- NCIT:C85504: Media
- NCIT:C14419: Strain
- NCIT:C120268: Inducer

For more information on representing cells, strains, plasmids, and genomes, see [Section 7.10.1](#)

7.9.3 Samples

A complete specification of a sample SHOULD be a [Component](#) that includes at least:

- A [SubComponent](#) instantiating each strain in the sample
- A [SubComponent](#) for the media or buffer
- A [SubComponent](#) for each additional reagent added to the media (e.g., inducers, antibiotics)
- [om:Measures](#) on each of these specifying the amount in the sample
- [om:Measures](#) on the [Component](#) for each environmental parameter (e.g., temperature, pH, culturing time)

7.9.4 Other Experimental Parameters

In order to deal with parameters associated with the context in general but not specific instances, e.g., temperature, pH, total sample volume, the [hasMeasure](#) property of [Identified](#) can be used. The [hasMeasure](#) of a [Component](#) provides context-free information (e.g., the pH of M9 media, the GC-content of a GFP coding sequence), while the [hasMeasure](#) of a material entity (SBO:0000240) [Feature](#) provides a measurement in context (e.g., the dosage of Arabinose in a sample).

Values of these parameters SHOULD be specified by attaching a [om:Measure](#) with a [type](#) set to the appropriate SBO term. The SBO terms that are RECOMMENDED as appropriate are members of the Systems Description Parameter (SBO:0000545) branch of SBO. Examples include:

- SBO:0000147: thermodynamic temperature (e.g., culturing at 27 C)
- SBO:0000332: half-life of an exponential decay (e.g., decay rate of a gRNA)
- SBO:0000304: pH (e.g., pH of M9 media)

7.10 Multicellular System Designs

SBOL has been used extensively to represent designs in homogeneous systems, where the same design is implemented in every cell. However, in recent years there has been increasing interest in multicellular systems, where biological designs are split across multiple cells to optimize the system behavior and function. Therefore, there is a need to define a set of best practices so that multicellular systems can be captured using SBOL in a standard way.

7.10.1 Representing Cell Types

To represent multicellular systems using SBOL, it is first necessary to represent cells. When doing so, it is important to be able to capture the following information: (i) taxonomy of the strain used, (ii) interactions occurring within cells of this type, and (iii) components inside the type of cell (e.g. genomes, plasmids). The approach RECOMMENDED in this section is capable of capturing this information, as shown in the example in [Figure 22](#). It uses a [Component](#) to represent a system that contains cells of the given type. The cells themselves are represented by a [SubComponent](#) inside the [Component](#), which is an [instanceOf](#) a [Component](#) capturing information about the species and strain of the cell in the design. This [Component](#) has a [type](#) of “cell” from the Gene Ontology (GO:0005623), and a [role](#) of “physical compartment” (SBO:0000290). Taxonomic information is captured by annotating the class instance with a URI for an entry in the NCBI Taxonomy Database.

As usual, other entities besides the cell that are relevant to the design are also captured as [Features](#). When these are contained within the cell, they are captured using a [Constraint](#) with restriction [contains](#) with the cell as [subject](#) and contained object as [object](#). Interactions which occur in this system are captured using the [Interaction](#) and [Participation](#) classes. Interactions which occur within the cell are specified by [Interaction](#) classes which contain the [SubComponent](#) instance representing the cell as a [participant](#) with a [role](#) of “physical compartment” (SBO:0000290).

7.10.2 Multiple Cell Types in a Single Design

The same approach can be extended to represent systems with multiple types of cells. The multicellular system can be represented as a [Component](#) that includes each strain of cell as a [SubComponent](#) that is an [instanceOf](#) a [Component](#) defining its strain. Interactions and constraints, such as a molecule that both strains interact with, are implemented using [ComponentReferences](#) to link to the definitions within each cell system description. An example is shown in [Figure 23](#).

7.10.3 Cell Ratios

The proportion of cell types present in a multicellular system can be captured using [om:Measure](#) on the representations of cells in the design. As a best practice, the value of these measure classes is a percentage less than or equal to 100%, representing the amount of a cell type present in the system compared to all other cell types present. Therefore, the sum of all these values specified in the system will typically be equal to 100%, though this may not be the case if the system is not completely defined. An example is shown in [Figure 24](#).

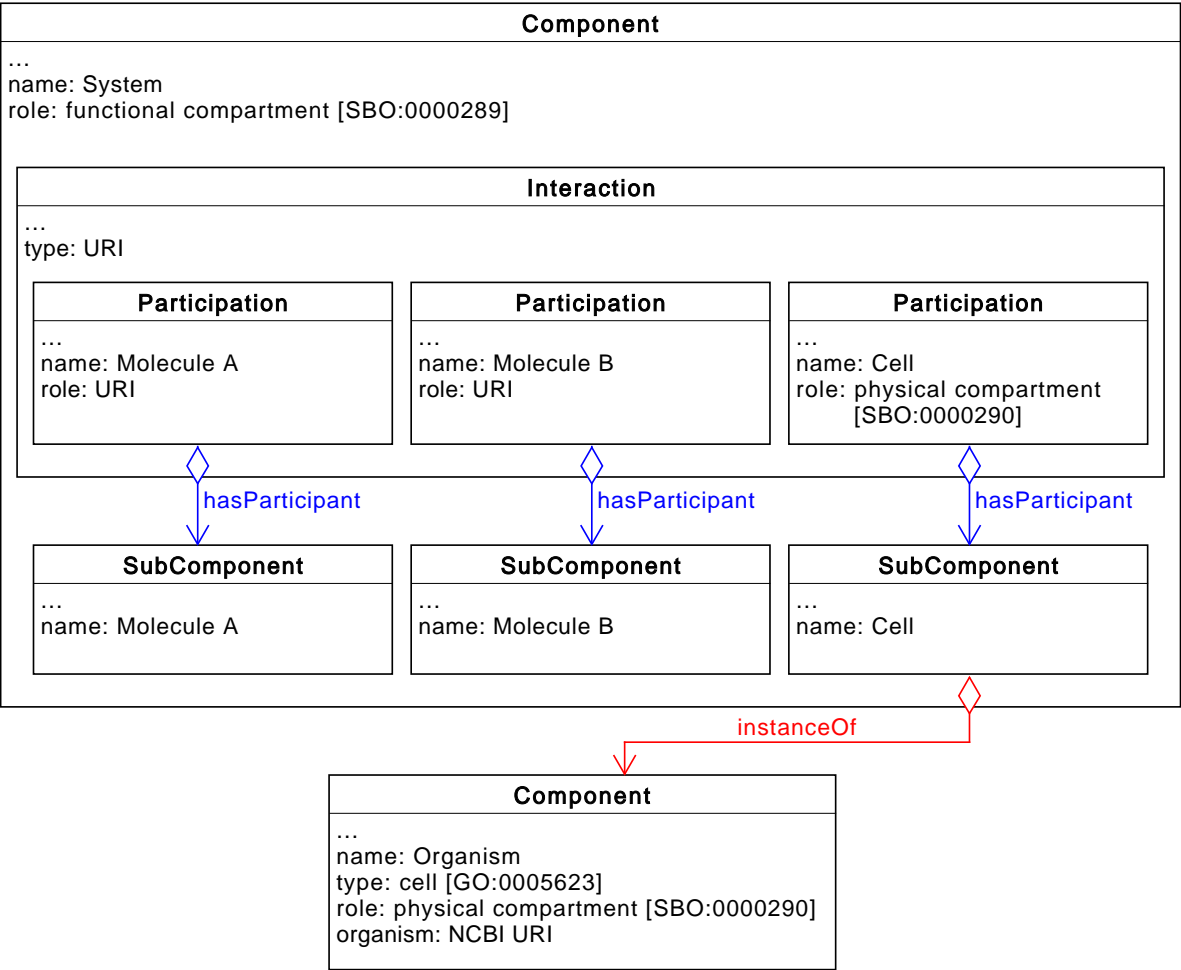


Figure 22: This is a proposed approach for capturing cell designs in SBOL. A **Component** annotated with a URI pointing to an entry in the NCBI Taxonomy Database is used to capture information about the cell’s strain/species. The **Component** has a type of “Cell” from the Gene Ontology (GO), and a role of “physical compartment”. Another **Component** is used to represent a system in which the cell is implemented. Entities, including the cell, are instantiated as **SubComponents**, and processes are captured using the **Interaction** class. Processes that are contained within the cell are represented by including the cell as a participant with a role of “physical compartment”.

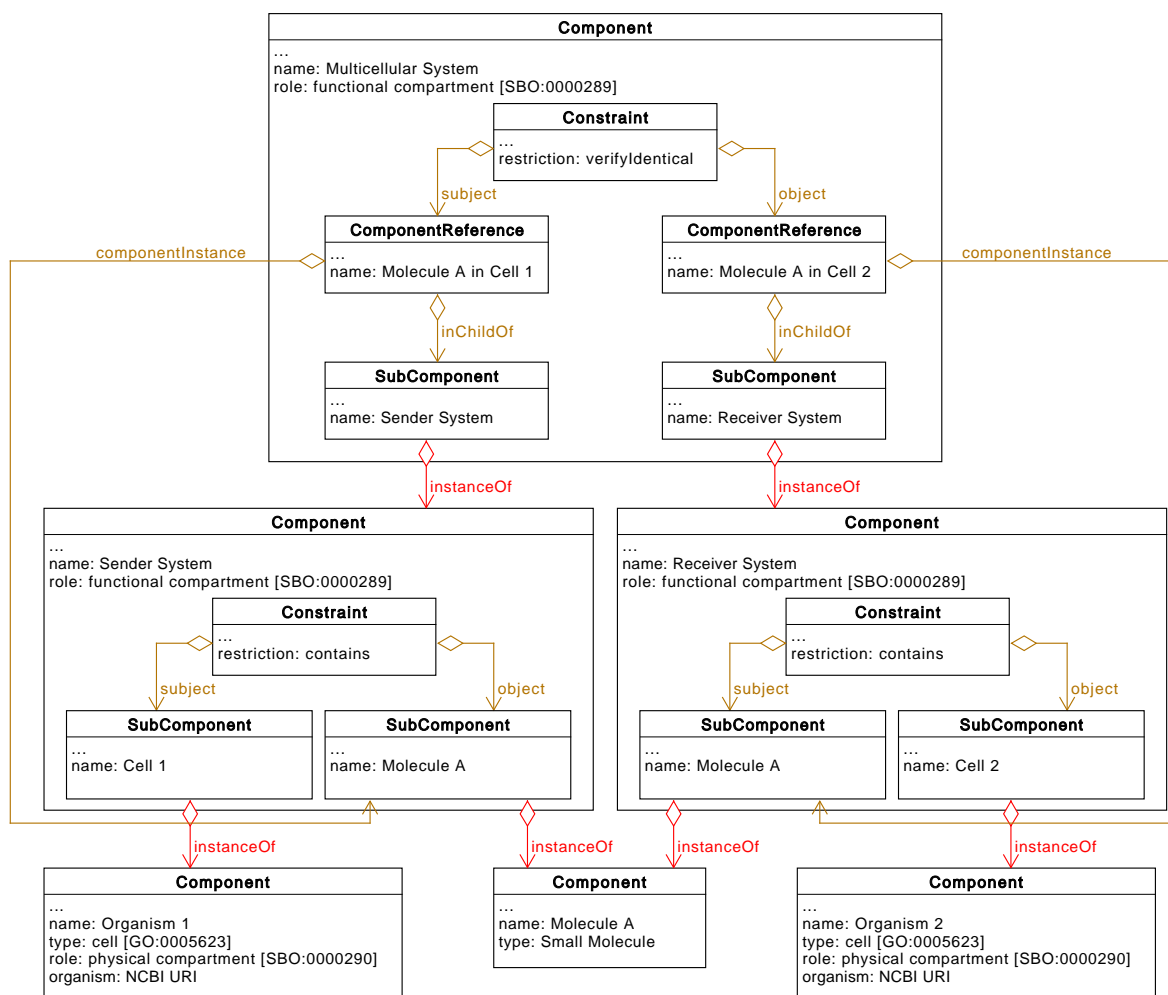


Figure 23: Captured here is a design involving two cells which both interact with the small molecule “Molecule A”. Designs for the sender and receiver systems are captured using constraint to show that each of these cells interacts with the Molecule A contained within it. The overall multicellular system is represented by a **Component** with a **role** of “functional compartment”, which is an SBO term. The two systems are included in this multicellular design as **SubComponents**, and the fact that Molecule A is shared between systems is indicated with a constraint.

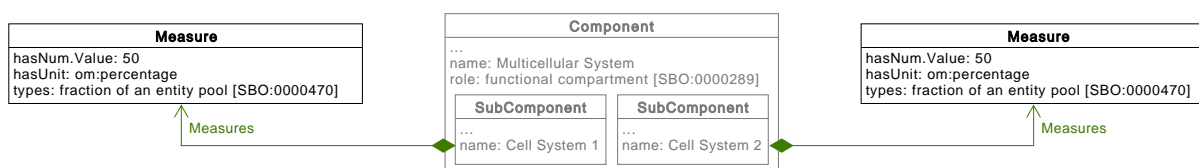


Figure 24: Annotating class instances with cellular proportions. Instances of the Measure class are used to capture the percentage of each cell type present in the multicellular system design.

8 SBOL RDF Serialization

In order for SBOL objects to be readily stored and exchanged, it is important that they are able to be *serialized*, i.e., converted to a sequence of bytes that can be stored in a file or exchanged over a network. The serialization format for SBOL is designed to meet several competing requirements. First, SBOL needs to support ad-hoc annotations and extensions. Second, SBOL needs to support processing by general database and semantic web software tools that have little or no knowledge of the SBOL data model. Finally, it ought to be relatively simple to write a new software implementation, so that SBOL can be readily used even in software environments where community-maintained implementations are not available.

To meet these goals, SBOL builds upon the Resource Description Framework (RDF). RDF is an abstract language for describing conceptual graph-oriented data models, and therefore does not mandate any specific serialization format. Instead, a number of different serialization formats are provided as separate specifications, such as RDF/XML, N-Triples, JSON-LD, and Turtle. These serialization formats are widely supported by RDF libraries such as *rdflib* for Python and Apache Jena for Java. For example, a simple SBOL definition of pLac can be serialized in RDF/XML as follows:

```
<?xml version="1.0" encoding="utf-8"?>
<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#" xmlns:sbol="http://sbols.org/v3#"
  <sbol:Component rdf:about="http://example.com#pLac">
    <sbol:name>pLac</sbol:name>
    <sbol:description>lactose inducible promoter</sbol:description>
    <sbol:sequence rdf:resource="http://example.com#sequence"/>
  </sbol:Component>
  <sbol:Sequence rdf:about="http://example.com#sequence">
    <sbol:encoding rdf:resource="http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html"/>
    <sbol:elements>caatacgcaaaccgcctctccccgcgcgttgccgattcattaatgcagctggcacga
caggtttcccgcactggaaagcgggcagtgagcgcaacgcaattaatgtgagttagctcactcattaggcaccacagg
ctttacactttatgcttccgctcgatgtgtgtggaattgtgagcggataacaatttcacaca</sbol:elements>
  </sbol:Sequence>
</rdf:RDF>
```

Alternatively, the same example can be serialized in Turtle as follows:

```
@prefix sbol: <http://sbols.org/v3#> .
@base <http://example.com#> .

<#pLac> a sbol:Component ;
  sbol:name "pLac" ;
  sbol:description "lactose inducible promoter" ;
  sbol:sequence <#sequence> .

<#sequence> a sbol:Sequence ;
  sbol:encoding <http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html> ;
  sbol:elements " "caatacgcaaaccgcctctccccgcgcgttgccgattcattaatgcagctggcacga
caggtttcccgcactggaaagcgggcagtgagcgcaacgcaattaatgtgagttagctcactcattaggcaccacagg
ctttacactttatgcttccgctcgatgtgtgtggaattgtgagcggataacaatttcacaca" " " .
```

The SBOL namespace, which is <http://sbols.org/v3#>, is used to indicate which entities and properties in the SBOL document are defined by SBOL. For example, the URI of the type `Component` is <http://sbols.org/v3#Component>. The SBOL namespace MUST NOT be used for any entities or properties not defined in this specification. Where possible, we have re-used predicates from widely-used terminologies (such as Dublin Core [DCMI Usage Board \(2012\)](#)) to expose as much of the data as practical to such standard RDF tooling.

9 SBOL Compliance

There are different types of software compliance with respect to the SBOL specification. First, a software tool can either support all classes of the SBOL 3 data model or only its structural subset. The structural subset includes the following classes:

- [Sequence](#)
- [Component](#)
 - [SubComponent](#)
 - [ComponentReference](#)
 - [LocalSubComponent](#)
 - [SequenceFeature](#)
 - [Location](#)
 - [Constraint](#)
- [Collection](#)

Second, an SBOL-compliant software tool can support import of SBOL, export of SBOL, or both. If it supports both import and export, it can do so in either a lossy or lossless fashion.

In order to test import compliance, developers are encouraged to use the SBOL test files found here:

<https://github.com/SynBioDex/SBOLTestSuite>

Examples of every meaningful subset of objects are provided, including both structural-only SBOL (that is, annotated DNA sequence data) and complete tests.

In order to test export compliance, developers are encouraged to validate SBOL files generated by their software with the SBOL Validator found here:

<https://validator.sbolstandard.org>

This validator can also be used to check lossless import/export support, since it can compare the data content of files imported and exported by a software tool.

Finally, developers of SBOL-compliant tools are encouraged to notify the SBOL editors (sbol-editors@googlegroups.com) when they have determined that their tool is SBOL compliant, so their tool can be publicly categorized as such on the SBOL website.

10 Mapping Between SBOL 1, SBOL 2, and SBOL3

In broad strokes, the SBOL 1 standard focused on conveying physical, structural information, whereas SBOL 2 expanded the scope to include functional aspects as well. The physical information about a designed genetic construct includes the order of its constituents and their descriptions. Specifying the exact locations of these constituents and their sequences allows genetic constructs to be defined unambiguously and reused in other designs. SBOL 2 extended SBOL 1 in several ways: it extends physical descriptions to include entities beyond DNA sequences, and it added support for functional descriptions of designs. SBOL 3 refines the SBOL 2 data model to simplify the representation of common use cases.

10.1 Mapping between SBOL 1 and SBOL 2

Figure 25 depicts the mapping of SBOL 1.1 classes to SBOL 2.x classes, indicating corresponding classes/properties by color. The SBOL 2.x **Model** and **ModuleDefinition** classes have no SBOL 1.1 equivalent, and thus are not shown. The mapping from SBOL 1.1 to SBOL 2.x proceeds as follows:

- SBOL 1.1 **Collection** objects containing **DnaComponent** objects map to SBOL 2.x **Collection** objects that contain **ComponentDefinition** objects with DNA **type** properties.
- SBOL 1.1 **DnaComponent** objects map to SBOL 2.x **ComponentDefinition** objects with DNA **type** properties.
- SBOL 1.1 **DnaSequence** objects map to an SBOL 2.x **Sequence** objects with **IUPAC DNA encoding** properties.
- SBOL 1.1 **SequenceAnnotation** objects with **bioStart** and **bioEnd** properties map to SBOL 2.x **SequenceAnnotation** objects that contain **Range** objects.
- SBOL 1.1 **SequenceAnnotation** objects that lack **bioStart** and **bioEnd** properties map to an SBOL 2.x **SequenceFeature** objects that contain **GenericLocation** objects.
- Each SBOL 1.1 **SequenceAnnotation** also maps to an SBOL 2.x **Component**, which represents the instantiation or usage of the appropriate **ComponentDefinition**.
- Each SBOL 1.1 **precedes** property maps to an SBOL 2.x **SequenceConstraint** that specifies a **precedes** restriction property.

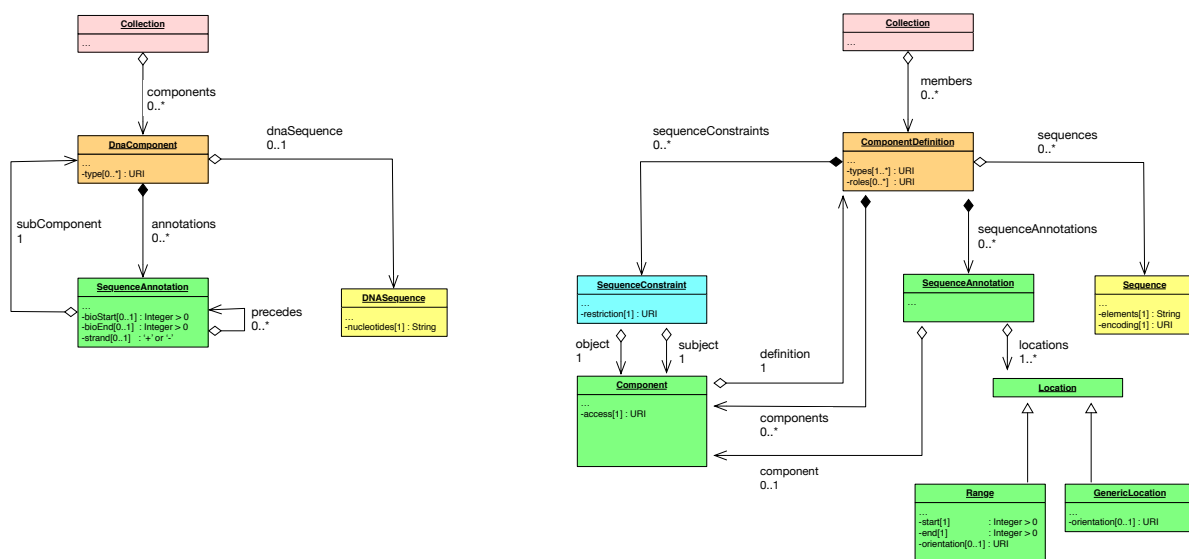
10.2 Mapping between SBOL 2 and SBOL 3

Figure 26 depicts the mapping of SBOL 2.3 classes to SBOL 3.x classes, indicating corresponding classes/properties by color. The SBOL 3.x **Namespace** class has no SBOL 2.x equivalent, and thus is not shown. The SBOL 2.x **Attachment**, **CombinatorialDerivation**, **ExperimentalData**, **Experiment**, **Implementation**, **Model**, **Participation**, **Sequence**, and **VariableComponent** classes are omitted or abstracted, since they are essentially unchanged in SBOL 3.x except for the following property renamings:

- In **Sequence**, the **encoding** property values for IUPAC map according to Table 17.
- In **VariableComponent**, the SBOL 2.x **operator** property maps to the SBOL 3.x **cardinality** property.
- In **Experiment**, the SBOL 2.x **experimentalData** property maps to the SBOL 3.x **member** property.

The mapping from SBOL 2.x to SBOL 3.x proceeds as follows:

- SBOL 2.x **ComponentDefinition** objects map to SBOL 3.x **Component** objects. The **type** property is mapped according to Table 18.



- SBOL 2.x **ModuleDefinition** objects map to SBOL 3.x **Component** objects with a **type** of **SBOL:00000241** (functional entity)
- Every **FunctionalComponent** in an SBOL 2.x **ModuleDefinition** with a "direction" property that is not "none" is listed in the **Interface** of its SBOL 3.x **Component**. The mapping from direction to interface properties is: "in" -> "inputs", "out" -> "outputs", "inout" -> "nondirectional". Finally, every Component with "access"="public" and "direction"="none" is listed as "nondirectional" in the Interface.
- Every **Component** in an SBOL 2.x **ComponentDefinition** with "access"="public" is listed as "nondirectional" in the **Interface** of its SBOL 3.x **Component**.
- SBOL 2.x **Component**, **Module**, and **FunctionalComponent** objects map to SBOL 3.x **SubComponent** objects
- SBOL 2.x **SequenceAnnotation** objects map to SBOL 3.x **SequenceFeature** objects if they do not have a **component**. If they do have a **component**, their locations are added to the corresponding SBOL3 **SubComponent**.
- SBOL 2.x **SequenceConstraint** objects map to SBOL 3.x **Constraint** objects
- SBOL 2.x **MapsTo** objects are converted by transforming each **MapsTo** into two SBOL 3.x objects: a **ComponentReference** and a **Constraint**.
 - For the **ComponentReference**, the **inChildOf** attribute of this **ComponentReference** attribute references the object that has the **MapsTo** as a child, and the **hasFeature** attribute references the object referred by the **remote** attribute from the **MapsTo** object.
 - The **Constraint** links this **ComponentReference** and the **SubComponent** referred to be the **local** attribute from the **MapsTo** object. The property values of the **Constraint** depend on the value of the **refinement** value for the **MapsTo** object:
 - ◆ If the refinement is **useRemote**, then the **restriction** is replaces, the **subject** is the **ComponentReference** and the **object** is the **SubComponent**.
 - ◆ If the refinement is **useLocal**, then the **restriction** is replaces, the **subject** is the **SubComponent** and the **object** is the **ComponentReference**.

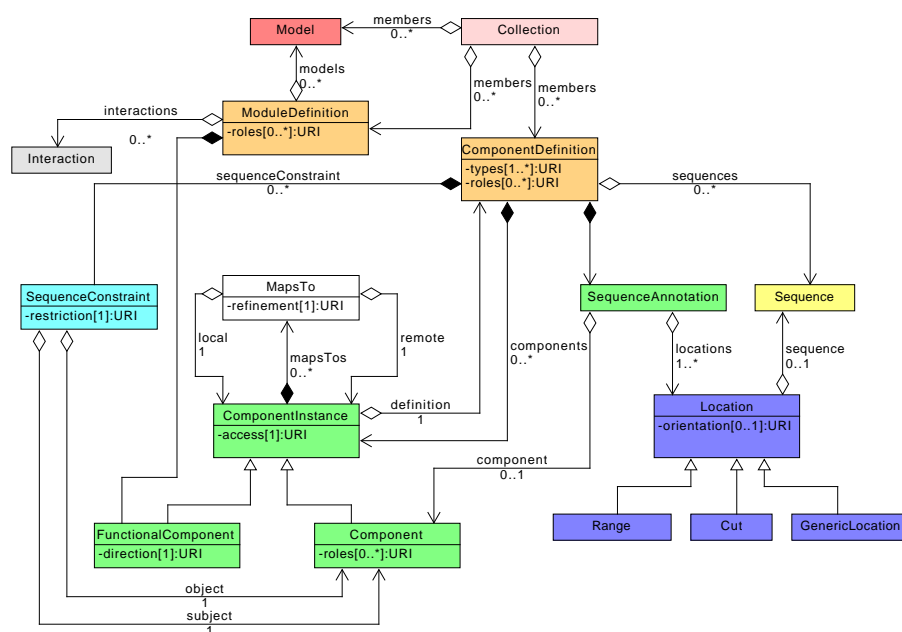
- ◆ If the refinement is **verifyIdentical**, then the **restriction** is **verifyIdentical**, the **subject** is the **ComponentReference** and the **object** is the **SubComponent**.
- ◆ The **merge refinement** was never well defined and rarely if ever used, so it has been removed from SBOL 3.x. If a **merge** is encountered, it SHOULD be handled as a **useRemote**.
- As an OPTIONAL optimization, if the **SubComponent** referred to by the **local** property of the **MapsTo** is a “placeholder” with no significant content apart from its **MapsTo** relationships, then it may be eliminated, all objects that pointed to it can point directly to the new **ComponentReference** instead, and all transitive constraints using it as a bridge reduced to link the endpoints directly.

SBOL 2.x Type	SBOL 3.x Type
http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html	http://sbols.org/v3#iupacNucleicAcid
http://www.chem.qmul.ac.uk/iupac/AminoAcid/	http://sbols.org/v3#iupacAminoAcid

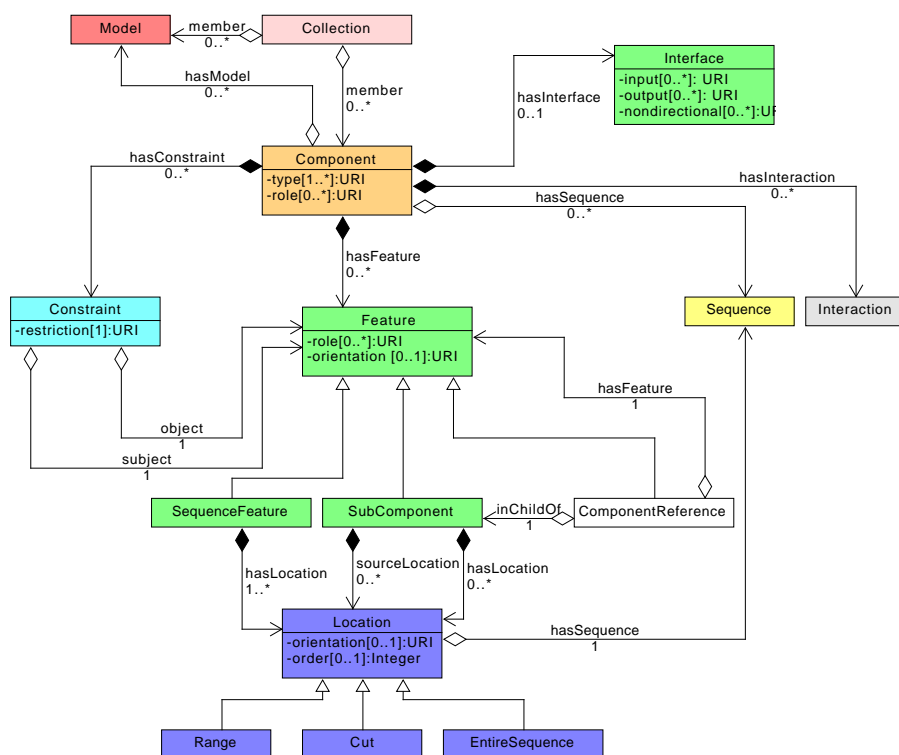
Table 17: Mapping of **Sequence encoding** values for IUPAC from SBOL2 to SBOL3

SBOL 2.x Type	SBOL 3.x Type
http://www.biopax.org/release/biopax-level3.owl#Dna	https://identifiers.org/SBO:0000251 (DNA)
http://www.biopax.org/release/biopax-level3.owl#DnaRegion	https://identifiers.org/SBO:0000251 (DNA)
http://www.biopax.org/release/biopax-level3.owl#Rna	https://identifiers.org/SBO:0000250 (RNA)
http://www.biopax.org/release/biopax-level3.owl#RnaRegion	https://identifiers.org/SBO:0000250 (RNA)
http://www.biopax.org/release/biopax-level3.owl#Protein	https://identifiers.org/SBO:0000252 (Protein)
http://www.biopax.org/release/biopax-level3.owl#SmallMolecule	https://identifiers.org/SBO:0000247 (Simple Chemical)
http://www.biopax.org/release/biopax-level3.owl#Complex	https://identifiers.org/SBO:0000253 (Non-covalent Complex)

Table 18: Mapping of SBOL2 **ComponentDefinition** types to SBOL3 **Component** types



(a) SBOL 2.3



(b) SBOL 3.x

Figure 26: The mapping from the SBOL 2.3 data model to the SBOL 3.x data model, indicating corresponding classes/properties by color.

References

- Biron, P. V., Permanente, K., and Malhotra, A. (2004). XML schema part 2: Datatypes second edition.
- Courtot, M., Juty, N., Knüpfer, C., Waltemath, D., Zhukova, A., Dräger, A., Dumontier, M., Finney, A., Golebiewski, M., Hastings, J., et al. (2011). Controlled vocabularies and semantics in systems biology. *Molecular systems biology*, 7(1):543.
- Cuellar, A. A., Lloyd, C. M., Nielsen, P. F., Bullivant, D. P., Nickerson, D. P., and Hunter, P. J. (2003). An overview of CellML 1.1, a biological model description language. *SIMULATION*, 79(12):740–747.
- DCMI Usage Board (2012). DCMI metadata terms. DCMI recommendation, Dublin Core Metadata Initiative.
- Degtyarenko, K., de Matos, P., Ennis, M., Hastings, J., Zbinden, M., McNaught, A., Alcántara, R., Darsow, M., Guedj, M., and Ashburner, M. (2008). ChEBI: a database and ontology for chemical entities of biological interest. *Nucleic Acids Research*, 36:D344–D350.
- Galdzicki, M., Clancy, K. P., Oberortner, E., Pocock, M., Quinn, J. Y., Rodriguez, C. A., Roehner, N., Wilson, M. L., Adam, L., Anderson, J. C., et al. (2014). The synthetic biology open language (SBOL) provides a community standard for communicating designs in synthetic biology. *Nature Biotechnology*, 32(6):545–550.
- Hucka, M. (2017). SBMLPkgSpec: a \LaTeX style file for SBML package specification documents. *BMC Research Notes*, 10(1):451.
- Hucka, M., Finney, A., Sauro, H. M., Bolouri, H., Doyle, J. C., Kitano, H., Arkin, A. P., Bornstein, B. J., Bray, D., Cornish-Bowden, A., Cuellar, A. A., Dronov, S., Gilles, E. D., Ginkel, M., Gor, V., Goryanin, I. I., Hedley, W. J., Hodgman, T. C., Hofmeyr, J.-H., Hunter, P. J., Juty, N. S., Kasberger, J. L., Kremling, A., Kummer, U., Nover, N. L., Loew, L. M., Lucio, D., Mendes, P., Minch, E., Mjolsness, E. D., Nakayama, Y., Nelson, M. R., Nielsen, P. F., Sakurada, T., Schaff, J. C., Shapiro, B. E., Shimizu, T. S., Spence, H. D., Stelling, J., Takahashi, K., Tomita, M., Wagner, J., Wang, J., and the rest of the SBML Forum (2003). The systems biology markup language (SBML): a medium for representation and exchange of biochemical network models. volume 19, pages 524–531. Oxford University Press (OUP).
- MathWorks (2015). MATLAB.
- Norrand, J., Kempe, T., and Messing, J. (1983). Construction of improved M13 vectors using oligodeoxynucleotide-directed mutagenesis. *Gene*, 26:101–106.
- Peccoud, J., Anderson, J. C., Chandran, D., Densmore, D., Galdzicki, M., Lux, M. W., Rodriguez, C. A., Stan, G.-B., and Sauro, H. M. (2011). Essential information for synthetic DNA sequences. *Nature Biotechnology*, 29(1):22–22.
- Roehner, N., Oberortner, E., Pocock, M., Beal, J., Clancy, K., Madsen, C., Misirli, G., Wipat, A., Sauro, H., and Myers, C. J. (2015). Proposed data model for the next version of the synthetic biology open language. *ACS Synthetic Biology*, 4(1):57–71.

A Complementary Standards

A.1 Adding Provenance with PROV-O

The PROV-O ontology (<https://www.w3.org/TR/prov-o/>) defines a complementary data model that is leveraged by SBOL to describe provenance. Provenance is central to a range of workflow management, quality control, and attribution tasks within the Synthetic Biology design process. Tracking attribution and derivation of one resource from another is paramount for managing intellectual property purposes. Source designs are often modified in systematic ways to generate derived designs, for example, by applying codon optimization or systematically removing all of a class of restriction enzyme sites. Documenting the transformation used, and any associated parameters, makes this explicit and potentially allows the process to be reproduced systematically. If a design has been used within other designs, and is later found to be defective, it is paramount that all uses of it, including uses of edited versions of the design, can be identified, and ideally replaced with a non-defective alternative. When importing data from external sources, it is important not only to attribute the original source (for example, GenBank), but also the tool used to perform the import, as this may have made arbitrary choices as to how to represent the source knowledge as SBOL. All these activities have in common that it is necessary to track what resource, and what transformation process was applied by whom to derive an SBOL design.

This section describes a minimal subset of PROV-O terms and classes that may be used by SBOL tools to support representation of provenance¹. Although the full-set of PROV-O terms can be used in SBOL documents, a subset of PROV-O is adopted as a best practice. It is advised that SBOL tools should at least understand this subset, defined in Figure 27. Providers of provenance information are free to make use of more of PROV-O than is described here. It is acceptable for tools that understand more than this subset to use as much as they are able. Tools that only understand this subset must treat any additional data as annotations. Tools that are not aware of SBOL provenance at all MUST maintain and provide access to this information as annotations. This specification does not state what the newly added properties must point to. As long as they are resources that are consistent with the PROV-O property domains, they are legal. For example, a [Component](#) may be derived from another [Component](#), but it would probably not make sense for it to be derived from a [Collection](#).

The most basic and general type of provenance relationship can be represented using the [prov:wasDerivedFrom](#) property. This relationship describes derivation of an SBOL entity from another. Any [Identified](#) object may be annotated with this property. More specific provenance relationships can also be defined using PROV-O, such as [prov:wasGeneratedBy](#). Generation of a new object is defined by the W3C PROV-O specification as follows:

...the completion of production of a new entity by an activity. This entity did not exist before generation and becomes available for usage after this generation.

These relationships are leveraged in SBOL tooling for describing multi-stage synthetic biology workflows.

Synthetic biology workflows may involve multiple stages, multiple users, multiple organizations, and interdisciplinary collaborations. These workflows can be described using four core PROV-O classes: [prov:Entity](#), [prov:Activity](#), [prov:Agent](#), and [prov:Plan](#). Any SBOL [Identified](#) object can implicitly act as an instance of PROV-O's [prov:Entity](#) class. Workflow histories (retrospective provenance) and workflow specifications (prospective provenance) can be described in SBOL using [prov:Activity](#) objects to link [Identified](#) objects into workflows. An [prov:Agent](#) (for example a software or a person) runs an [prov:Activity](#) according to a [prov:Plan](#) to generate new entities. Resources representing [prov:Agent](#), [prov:Activity](#) and [prov:Plan](#) classes should be handled as [TopLevel](#), whilst [prov:Usage](#) and [prov:Association](#) resources should be treated as child [Identified](#) objects within their parent [prov:Activity](#) objects.

A design-build-test-learn SBOL ontology has been adopted for use with PROV-O classes (see Table 19). The terms *design*, *build*, *test*, and *learn* provide a high level workflow abstraction that allows tool-builders to quickly search for

¹ We thank Dr Paolo Missier from the School of Computing Science, Newcastle University for discussions regarding the use of PROV-O.

and isolate provenance histories relevant to their domain, while keeping track of the flow of data between different users working in different domains of synthetic biology. These terms SHOULD BE used on the `type` property of the `prov:Activity` class. (Note that this property is a special property added by the SBOL specification, and is not part of the original PROV-O specification.) Additionally, these terms SHOULD BE used in the `prov:hadRole` properties on `prov:Usage` to qualify how the referenced `prov:entity` is used by the parent `prov:Activity`. Logical constraints are placed on the order in which different types of `prov:Activity`s are chained into design-build-test-learn workflows. These rules additionally place constraints on the types of objects that may be used as inputs for a particular type of `prov:Activity`. For example, a *design* `prov:Usage` may be used as an input for either a *design* or *build* `prov:Activity` but MUST NOT be used as an input for a *test* `prov:Activity`. An example of how these terms are used is provided in Figure 28.

Activity Type	URI	Description
Design	http://sbols.org/v3#design	Design describes the process by which a conceptual representation of an engineer's imagined and intended design for a biological system is created or derived.
Build	http://sbols.org/v3#build	Build describes the process by which a biological construct, sample, or clone is implemented in the laboratory.
Test	http://sbols.org/v3#test	Test describes the process of performing experimental measurements to characterize a synthetic biological construct.
Learn	http://sbols.org/v3#learn	Learn describes the process of analyzing experimental measurements to produce a new entity that represents biological knowledge.

Table 19: Synthetic biology workflow ontology

In addition to the design-build-test-learn terms, users may also wish to include more specific terms to specify how SBOL objects are used in-house in their own recipes, protocols, or computational analyses. In fact, it is expected that the SBOL workflow ontology will be expanded over time, as users experiment with and develop their own custom ontologies. For now, however, it is RECOMMENDED that SBOL tools also include the high-level terms in Table 19 to support data exchange across interdisciplinary boundaries.

A.1.1 `prov:Activity`

A generated `prov:Entity` is linked through a `prov:wasGeneratedBy` relationship to an `prov:Activity`, which is used to describe how different `prov:Agents` and other entities were used. An `prov:Activity` is linked through a `prov:qualifiedAssociation` to `prov:Associations`, to describe the role of agents, and is linked through `prov:qualifiedUsage` to `prov:Usages` to describe the role of other entities used as part of the activity. Moreover, each `prov:Activity` includes optional `prov:startedAtTime` and `prov:endedAtTime` properties. When using `prov:Activity` to capture how an entity was derived, it is expected that any additional information needed will be attached as annotations. This may include software settings or textual notes. Activities can also be linked together using the `prov:wasInformedBy` relationship to provide dependency without explicitly specifying start and end times.

The `type` property

An `prov:Activity` MAY have one or more `type` properties, each of type `URI` that explicitly specifies the type of the provenance `prov:Activity` in more detail. If specified, it is RECOMMENDED that at least one `type` property refers to a `URI` from Table 19.

The `prov:startedAtTime` property

The `prov:startedAtTime` property is OPTIONAL and contains a `DateTime` (see Section 7.7) value, indicating when the activity started. If this property is present, then the `prov:endedAtTime` property is REQUIRED.

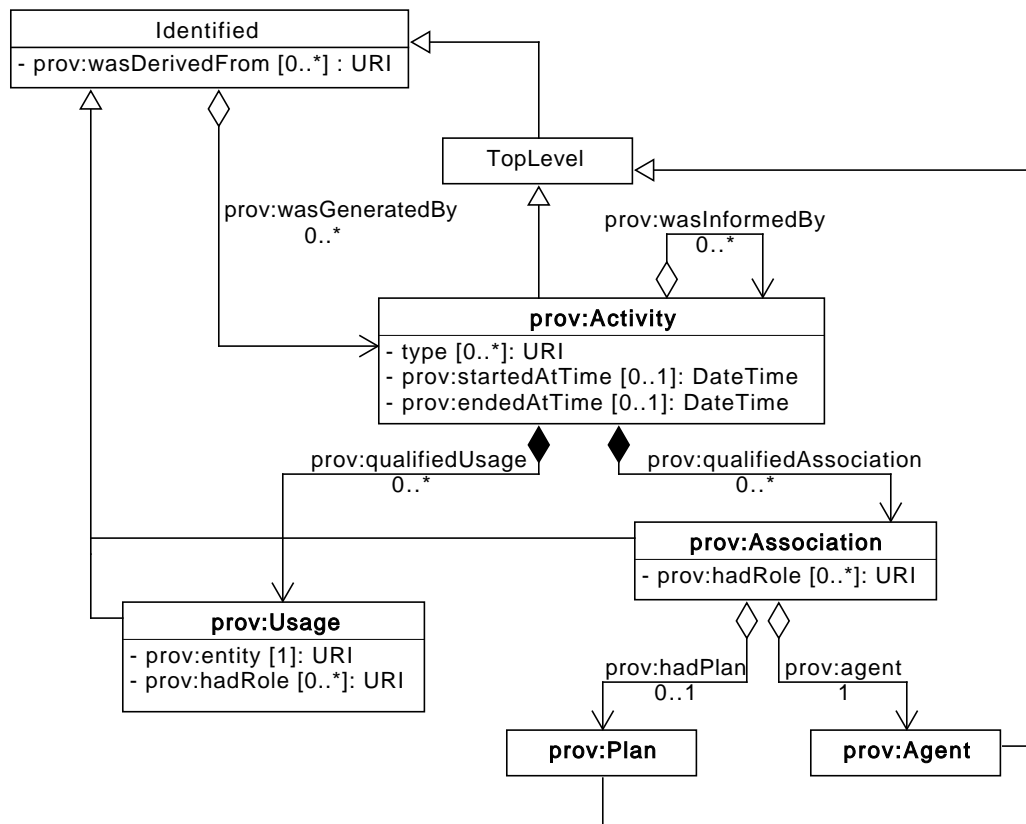


Figure 27: Relationships between SBOL and PROV-O classes. The PROV-O classes `prov:Activity`, `prov:Plan`, and `prov:Agent` all derive from `TopLevel` in the context of the SBOL data model.

The `prov:endedAtTime` property

The `prov:endedAtTime` property is OPTIONAL and contains a `DateTime` (see [Section 7.7](#)) value, indicating when the activity ended.

The `prov:qualifiedAssociation` property

An `prov:Activity` MAY have one or more `prov:qualifiedAssociation` properties, each of type `URI` that refers to an `prov:Association` object.

The `prov:qualifiedUsage` property

An `prov:Activity` MAY have one or more `prov:qualifiedUsage` properties, each of type `URI` that refers to an `prov:Usage` object.

The `prov:wasInformedBy` property

An `prov:Activity` MAY have one or more `prov:wasInformedBy` properties, each of type `URI` that refers to another `prov:Activity` object.

A.1.2 *prov:Usage*

How different entities are used in an *prov:Activity* is specified with the *prov:Usage* class, which is linked from an *prov:Activity* through the *prov:Usage* relationship. A *prov:Usage* is then linked to an *prov:Entity* through the *prov:entity* property *URI* and the *prov:hadRole* property species how the *prov:Entity* is used. When the *prov:wasDerivedFrom* property is used together with the full provenance described here, the entity pointed at by the *prov:wasDerivedFrom* property MUST be included in a *prov:Usage*.

The prov:entity property

The *prov:entity* property is REQUIRED and MUST contain a *URI* which MAY refer to an *Identified* object.

The prov:hadRole property

An *prov:Usage* MAY have one or more *prov:hadRole* properties, each of type *URI* that refers to particular term(s) describing the usage of an *prov:Entity* referenced by the *prov:entity* property. Recommended terms that are defined in Table 19 can be used to indicate how the referenced *prov:Entity* is being used in this *prov:Activity*.

A.1.3 *prov:Association*

An *prov:Association* is linked to an *prov:Agent* through the *prov:agent* relationship. The *prov:Association* includes the *prov:hadRole* property to qualify the role of the *prov:Agent* in the *prov:Activity*.

The prov:agent property

The *prov:agent* property is REQUIRED and MUST contain a *URI* that refers to an *prov:Agent* object.

The prov:hadRole property

An *prov:Association* MAY have one or more *prov:hadRole* properties, each of type *URI* that refers to particular term(s) that describes the role of the *prov:Agent* in the parent *prov:Activity*.

The prov:hadPlan property

The *prov:hadPlan* property is OPTIONAL and contains a *URI* that refers to a *prov:Plan*.

A.1.4 *prov:Plan*

The *prov:Plan* entity can be used as a place holder to describe the steps (for example scripts or lab protocols) taken when an *prov:Agent* is used in a particular *prov:Activity*.

A.1.5 *prov:Agent*

Examples of agents are a person, organization, or software tool. These agents should be annotated with additional information, such as software version, needed to be able to run the same *prov:Activity* again.

Example - Codon optimization

Codon optimization is an example of where provenance properties can be applied. The relationship between an original CDS and the codon-optimized version could simply be represented using the *prov:wasDerivedFrom* predicate, in a light-weight form. With more comprehensive use of the PROV ontology, the codon optimization can be represented as an *prov:Activity*. This *prov:Activity* can then include additional information, such as the *prov:Agent* responsible (in this case, codon-optimizing software), and additional parameters.

Example - Deriving strains

Bacterial strains are often derived from other strains through modifications such as gene knockouts or mutations. For example, the *Bacillus subtilis* 168 strain was derived from the NCIMB3610 strain in the 1940s through x-radiation.

B. subtilis 168 is a laboratory strain and has several advantages as a model organism in synthetic biology. The relationship between the original strain and the 168 strain can be represented using the `prov:wasDerivedFrom` predicate or, more comprehensively, with an `prov:Activity` describing the protocols used.

Example - Design-build-test-learn Workflow

Figure 28 illustrates one complete iteration through a design-build-test-learn cycle. The workflow begins with a **Model** which describes the hypothesized behavior of a biological device. Using a computational tool, a new Design (**Component**) is composed from biological parts, which links back to its **Model**. A genetic construct is then produced in the laboratory via an assembly protocol, and this biological sample is represented by a Build (**Implementation**). Once constructed, the Build is then characterized in the laboratory using an automated measurement protocol on a Tecan plate reader, thus generating Test data (represented by an **ExperimentalData**). Finally, a new **Model** is derived from these data using a fitting algorithm implemented in the Python programming language. The final **Model** may not match the beginning **Model**, as the observed behavior may not match the prediction.

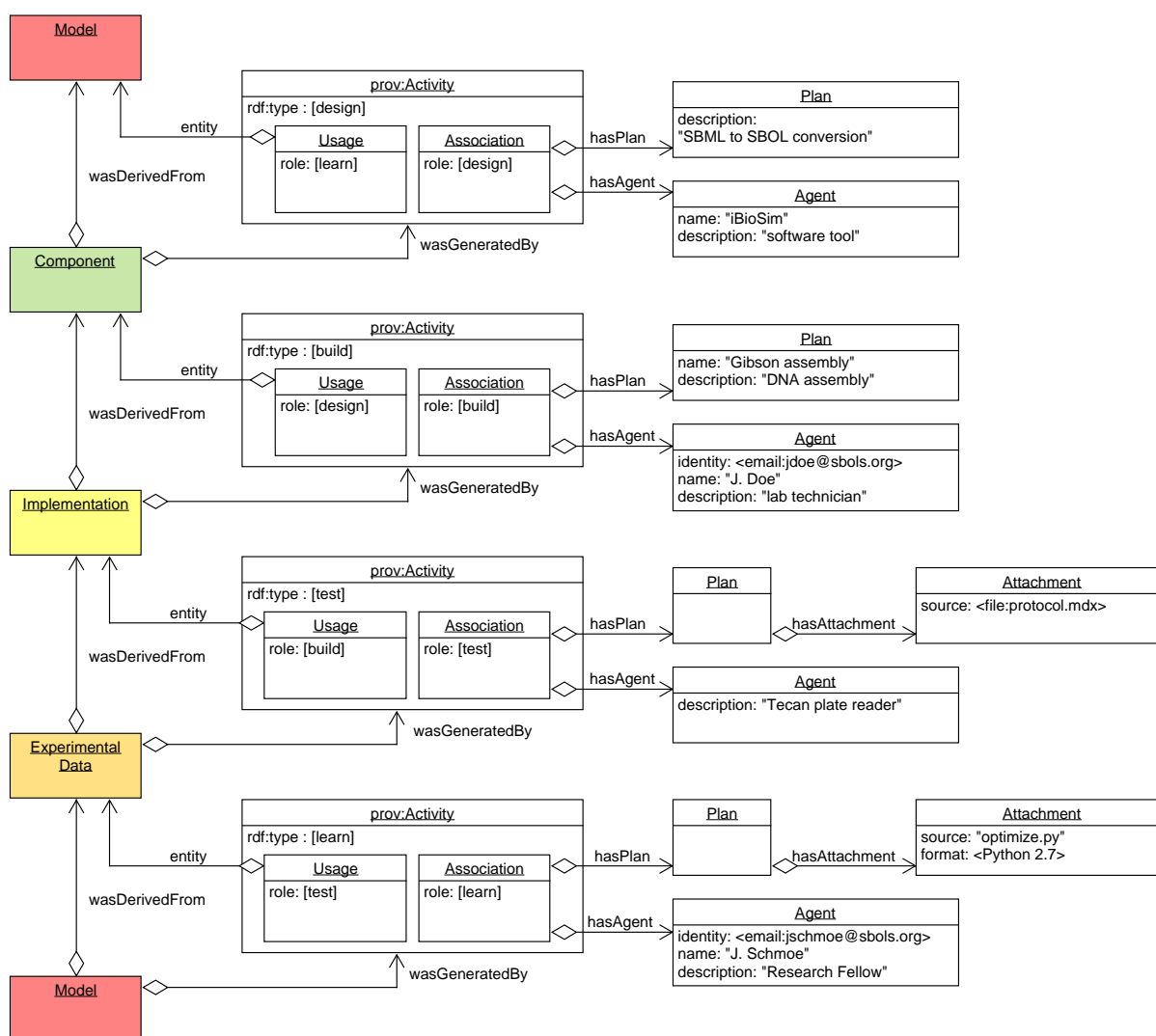


Figure 28: An example data structure representing an idealized workflow for model-based design.

Example - Combinatorial Derivation

As specified in the description of [CombinatorialDerivation](#), provenance can be used to link each generated [Component](#) (or [Collection](#) thereof) back to the source form which it was derived. In particular, each derived design links with [prov:wasDerivedFrom](#) to the [CombinatorialDerivation](#) that it was derived from. Also, each [SubComponent](#) has a [prov:wasDerivedFrom](#) linking it to the [SubComponent](#) within the [template](#) that it is derived from. The advantage of these provenance links is that they provide sufficient information to validate that this derived design has been properly derived from the specified [CombinatorialDerivations](#).

A.2 Adding Measures/Parameters with OM

There are at least two well-established cases for including measures/parameters and their associated units in SBOL design specifications. These use cases are the specification of genetic circuit designs and their associated parameters (such as rates of transcription) and the specification of environmental conditions for biological system designs (such as growth media concentrations and temperatures). In the first use case, parameters are necessary to enable the generation of quantitative models of circuit behavior from circuit design specifications. In the second use case, measures are necessary to define experimental conditions and enable the analysis of system behavior or characterization with respect to environmental context.

The Ontology of Units of Measure (OM) (<http://www.ontology-of-units-of-measure.org/resource/om-2>) already defines a data model for representing measures and their associated units. Here, a subset of OM is adopted by SBOL to describe these concepts for biological design specifications. As shown in [Figure 29](#), SBOL leverages three of the base classes defined by the OM: [om:Measure](#), [om:Unit](#) and [om:Prefix](#). A [om:Measure](#) links a numerical value to a [om:Unit](#), which may or may not have a [om:Prefix](#) (e.g. centi, milli, micro, etc.). As these classes are adopted by SBOL, [om:Measure](#) is treated as a subclass of [Identified](#), while [om:Unit](#) and [om:Prefix](#) are treated as subclasses of [TopLevel](#). In addition, SBOL adopts the following OM [om:Unit](#) subclasses: [om:SingularUnit](#), [om:CompoundUnit](#), [om:UnitMultiplication](#), [om:UnitDivision](#), [om:UnitExponentiation](#), and [om:PrefixedUnit](#). Lastly, SBOL adopts the following [om:Prefix](#) subclasses from OM: [om:SIPrefix](#) and [om:BinaryPrefix](#).

SBOL-compliant tools are allowed to read, write, and modify data belonging to OM classes other than those described here, but this specification does not provide any guidance for the interpretation or use of these data in the context of SBOL.

A.2.1 om:Measure

The purpose of the [om:Measure](#) class is to link a numerical value to a [om:Unit](#).

The om:hasNumericalValue property

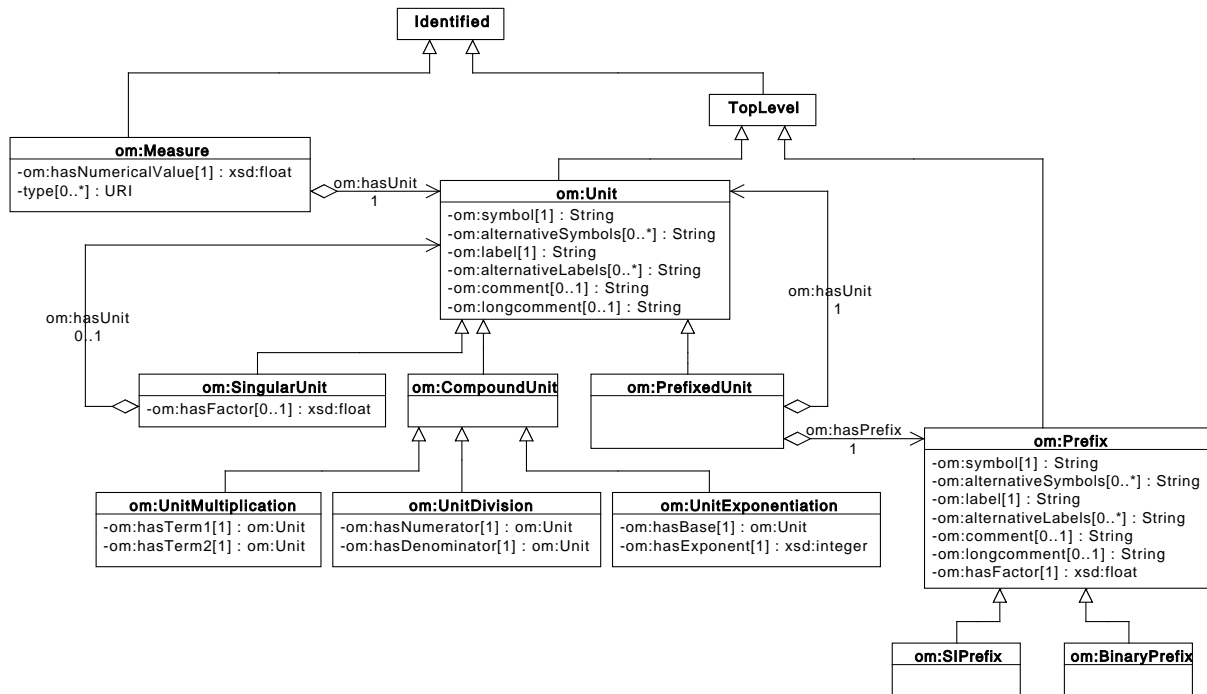
The [om:hasNumericalValue](#) property is REQUIRED and MUST contain a single `xsd:float`.

The om:hasUnit property

The [om:hasUnit](#) property is REQUIRED and MUST contain a [URI](#) that refers to a [om:Unit](#). The OM provides [URIs](#) for many existing instances of the [om:Unit](#) class for reference (for example, <http://www.ontology-of-units-of-measure.org/resource/om-2/gramPerLitre>).

The type property

A [om:Measure](#) MAY have one or more [type](#) properties, each is of type [URI](#). It is RECOMMENDED that one of these [URIs](#) identify a term from the Systems Description Parameter branch of the Systems Biology Ontology (SBO) (<http://www.ebi.ac.uk/sbo/main/>). This [type](#) property of the [om:Measure](#) class is not specified in the OM and is added by SBOL to describe different types of parameters (for example, rate of reaction is identified by the SBO term <http://identifiers.org/biomodels.sbo/SBO:0000612>).

Figure 29: OM classes adopted by SBOL and their subclass relationships to [Identified](#) and [TopLevel](#)

A.2.2 *om:Unit*

As adopted by SBOL, [om:Unit](#) is an abstract class that is extended by other classes to describe units of measure using a shared set of properties.

The *om:symbol* property

The [om:symbol](#) property is REQUIRED and MUST contain a [String](#). This [String](#) is commonly used to abbreviate the unit of measure's name. For example, the unit of measure named "gram per liter" is commonly abbreviated using the [String](#) "g/l".

The *om:alternativeSymbols* property

The [om:alternativeSymbols](#) property is OPTIONAL and MAY contain a set of [Strings](#). This property can be used to specify alternative abbreviations other than that specified using the [om:symbol](#) property.

The *om:label* property

The [om:label](#) property is REQUIRED and MUST contain a [String](#). This [String](#) is a common name for the unit of measure and SHOULD be identical to any [String](#) contained by the [name](#) property inherited from [Identified](#).

The *om:alternativeLabels* property

The [om:alternativeLabels](#) property is OPTIONAL and MAY contain a set of [Strings](#). This property can be used to specify alternative common names other than that specified using the [om:label](#) property.

The *om:comment* property

The [om:comment](#) property is OPTIONAL and MAY contain a [String](#). This [String](#) is a description of the unit of measure and SHOULD be identical to any [String](#) contained by the [description](#) property inherited from [Identified](#).

The om:longcomment property

The `om:longcomment` property is OPTIONAL and MAY contain a `String`. This `String` is a long description of the unit of measure and SHOULD be longer than any `String` contained by the `om:comment` property.

A.2.3 om:SingularUnit

The purpose of the `om:SingularUnit` class is to describe a unit of measure that is not explicitly represented as a combination of multiple units, but could be equivalent to such a representation. For example, a joule is considered to be a `om:SingularUnit`, but it is equivalent to the multiplication of a newton and a meter.

The om:hasUnit property

The `om:hasUnit` is OPTIONAL and MAY contain a `URI`. This `URI` MUST refer to another `om:Unit`. The `om:hasUnit` property can be used in conjunction with the `om:hasFactor` property to specify whether a `om:SingularUnit` is equivalent to another `om:Unit` multiplied by a factor. For example, an angstrom is equivalent to 10^{-10} meters.

The om:hasFactor property

The `om:hasFactor` property is OPTIONAL and MAY contain a `xsd:float`. If the `om:hasFactor` property of a `om:SingularUnit` is non-empty, then its `om:hasUnit` property SHOULD also be non-empty.

A.2.4 om:CompoundUnit

As adopted by SBOL, `om:CompoundUnit` is an abstract class that is extended by other classes to describe units of measure that can be represented as combinations of multiple other units of measure.

A.2.5 om:UnitMultiplication

The purpose of the `om:UnitMultiplication` class is to describe a unit of measure that is the multiplication of two other units of measure.

The om:hasTerm1 property

The `om:hasTerm1` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`. This `om:Unit` is the first multiplication term.

The om:hasTerm2 property

The `om:hasTerm2` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`. This `om:Unit` is the second multiplication term. It is okay if the `om:Unit` referred to by `om:hasTerm1` is the same as that referred to by `om:hasTerm2`.

A.2.6 om:UnitDivision

The purpose of the `om:UnitDivision` class is to describe a unit of measure that is the division of one unit of measure by another.

The om:hasNumerator property

The `om:hasNumerator` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`.

The om:hasDenominator property

The `om:hasDenominator` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`.

A.2.7 *om:UnitExponentiation*

The purpose of the `om:UnitExponentiation` class is to describe a unit of measure that is raised to an integer power.

The `om:hasBase` property

The `om:hasBase` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`.

The `om:hasExponent` property

The `om:hasExponent` property is REQUIRED and MUST contain an `xsd:integer`.

A.2.8 *om:PrefixedUnit*

The purpose of the `om:PrefixedUnit` class is to describe a unit of measure that is the multiplication of another unit of measure and a factor represented by a standard prefix such as “milli,” “centi,” “kilo,” etc.

The `om:hasUnit` property

The `om:hasUnit` property is REQUIRED and MUST contain a `URI` that refers to another `om:Unit`.

The `om:hasPrefix` property

The `om:hasPrefix` property is REQUIRED and MUST contain a `URI` that refers to a `om:Prefix`.

A.2.9 *om:Prefix*

As adopted by SBOL, `om:Prefix` is an abstract class that is extended by other classes to describe factors that are commonly represented by standard unit prefixes. For example, the factor 10^{-3} is represented by the standard unit prefix “milli.”

The `om:symbol` property

The `om:symbol` property is REQUIRED and MUST contain a `String`. This `String` is commonly used to abbreviate the name of the unit prefix. For example, the `String` “m” is commonly used to abbreviate the name “milli.”

The `om:alternativeSymbols` property

The `om:alternativeSymbols` property is OPTIONAL and MAY contain a set of `Strings`. This property can be used to specify alternative abbreviations other than that specified using the `om:symbol` property.

The `om:label` property

The `om:label` property is REQUIRED and MUST contain a `String`. This `String` is a common name for the unit prefix and SHOULD be identical to any `String` contained by the `name` property inherited from `Identified`.

The `om:alternativeLabels` property

The `om:alternativeLabels` property is OPTIONAL and MAY contain a set of `Strings`. This property can be used to specify alternative common names other than that specified using the `om:label` property.

The `om:comment` property

The `om:comment` property is OPTIONAL and MAY contain a `String`. This `String` is a description of the unit prefix and SHOULD be identical to any `String` contained by the `description` property inherited from `Identified`.

The `om:longcomment` property

The `om:longcomment` property is OPTIONAL and MAY contain a `String`. This `String` is a long description of the unit of measure and SHOULD be longer than any `String` contained by the `om:comment` property.

The `om:hasFactor` property

The `om:hasFactor` property is REQUIRED and MUST contain an `xsd:float`.

A.2.10 `om:SIPrefix`

The purpose of the `om:SIPrefix` class is to describe standard SI prefixes such as “milli,” “centi,” “kilo,” etc.

A.2.11 `om:BinaryPrefix`

The purpose of the `om:BinaryPrefix` class is to describe standard binary prefixes such as “kibi,” “mebi,” “gibi,” etc. These prefixes commonly precede units of information such as “bit” and “byte.”

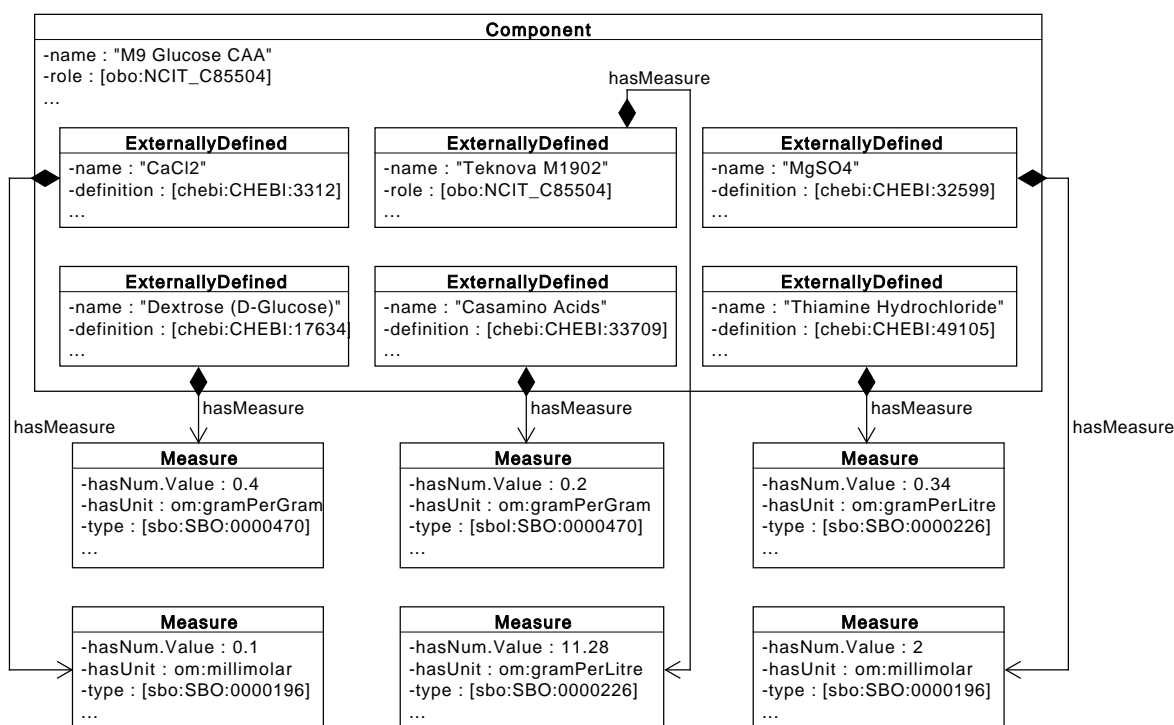


Figure 30: Growth media recipe represented using instances of the `om:Measure` and `om:Unit` classes from the OM.