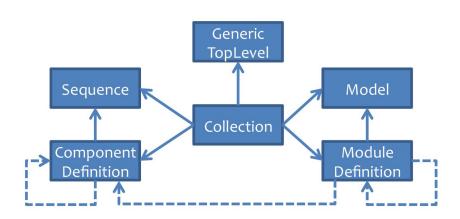
Introduction to libSBOLj and sboljs

Chris J. Myers

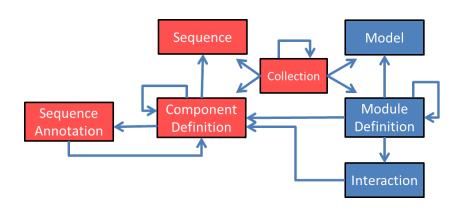
University of Utah

SBOL Workshop August 11, 2017

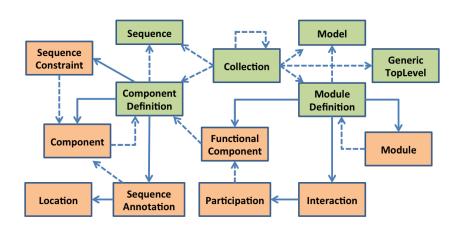
SBOL 2 Data Model



SBOL 2 Data Model



SBOL 2 Data Model



SBOL Libraries

- Crucial to the success of a standard is software infrastructure to support developers' integration of the standard within their tools.
- There are several library implementations of the SBOL data structure, which provide an application programmers interface (API) for tool developers to interact with SBOL data objects.
 - libSBOLj native Java library
 - sboljs Javascript library
 - libSBOL C/C++ library
 - pySBOL Python library

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 - libSBOL C/C++ library
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libSBOLj - native Java SBOL Library

- Library available from Maven central:
 - Group Id org.sbolstandard
 - Artifact Id libSBOLj
 - Version 2.2.1
- Distribution includes detailed documentation for the class definitions and the methods provided by the API.
- Supports validation/conversion to/from FASTA, GenBank, and SBOL1.
- Includes support to search, fetch, and submit designs to SynBioHub.
- Utilized by an online validator/converter available from the SBOL website, and it also provides a webservice to be used by non-java applications.

SBOL Documents

- libSBOLj organizes all SBOL data within an SBOLDocument.
- Includes a list of each type of top level object:
 - Collections.
 - ModuleDefinitions.
 - ComponentDefinitions,
 - Sequences,
 - Models, and
 - GenericTopLevel objects.
- These lists are organized to allow for easy search by their unique reference identifiers (URIs) and validation that they are distinct.
- libSBOLj includes methods for creating, updating, accessing, and removing these data objects, as well as, their child objects.

Creating an SBOLDocument

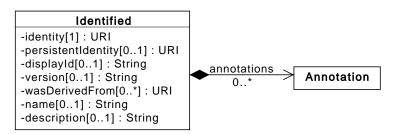
```
String uriPrefix = "http://cellocad.org/";
SBOLDocument document = new SBOLDocument();
document.setDefaultURIprefix(uriPrefix);
document.setComplete(true);
document.setCreateDefaults(true);
```

- Default URI prefix prefix to use when none provided to create method.
- Complete ensure that all URI references point to valid SBOL objects.
- Create defaults implicitly create ComponentInstances as needed.

Understanding UML Diagrams

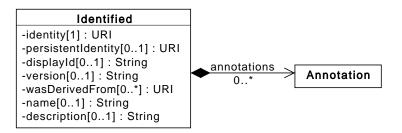
- Classes represented as boxes labeled with their member variables with types and cardinalities.
- Arrows with cardinality indicate associations between classes.
- A hollow diamond at the origin of an arrow represents shared aggregation (i.e., object is referenced and not owned).
- A solid diamond at the origin of an arrow represents composite aggregation (i.e., child object is owned by its parent object).
- Hollow arrows are used to represent inheritance.

Identified (Base Class for All SBOL Objects)



- identity globally unique URI to identify this object (required).
- persistentIdentity identity shared by multiple versions of the same object (optional).
- displayId human-readable id composed of alphanumeric and underscore characters (optional).
- version uses semantic versioning to identify multiple versions of the same object (optional).

Identified (Base Class for All SBOL Objects)



- wasDerivedFrom identities of objects that this is derived from (optional).
- name human-readable String of arbitrary characters (optional).
- description thorough text description of the object (optional).
- annotations additional data about this object (more later).

Compliant Top-Level URIs

$$\langle \mathit{URI}\ \mathit{prefix} \rangle / \langle \mathit{displayId} \rangle / \langle \mathit{version} \rangle$$

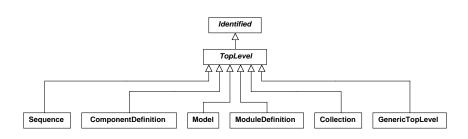
- The identity MUST begin with a URI prefix that maps to a domain over which the user has control.
- The persistentIdentity and displayId properties are REQUIRED.
- The persistentIdentity MUST end with a delimiter ('/', '#', or ':') followed by the displayId of the object.
- If an object is not given a version, then its identity and persistentIdentity properties MUST contain the same URI.
- If an object has a version, then its identity property MUST contain a URI of the form \(\langle persistent \text{Identity} \rangle \langle version \rangle ".

Compliant Child URIs

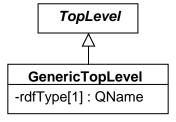
 $\langle parent\ persistent | dentity \rangle / \langle display | d \rangle / \langle parent\ version \rangle$

- The persistentIdentity MUST begin with the persistentIdentity of its parent object and be immediately followed by a delimiter ('/', '#', or ':') and the displayId of the object.
- The version MUST contain the same String as the version property of the object's parent object.

TopLevel



GenericTopLevel



GenericTopLevel Objects and Annotations

- Software tools that need to store data that is not encoded within SBOL can do so using GenericTopLevel objects and custom Annotations.
- When the library reader encounters a tag for a TopLevel object that it does not recognize, this data is stored within a GenericTopLevel object.
- Within TopLevel objects, when a tag is not recognized the data is stored within a custom Annotation object.
- Tools using our library that do not recognize this data will round-trip it unmodified when writing an SBOL file.
- Tools that would like to make use of this data can interpret and manipulate the raw data, which is stored in a tree-like data structure.

Creating SBOL Data Objects

- SBOLDocument class includes create methods for each TopLevel object.
 - displayld only URI prefix taken from default, no version
 - displayId, version URI prefix taken from default
 - URIprefix, displayId, version
- All required fields are also parameters to these create methods.

create (TopLevel) (URIprefix, displayId, version, (required fields))

Setting and Editing Optional Fields

Methods to set/unset each optional field, as well as check if isSet.

```
genericTopLevel.setName("Cello_UCF_to_SBOL_conversion");
genericTopLevel.setDescription("Conversion_of_the_Cello_UCF_parts_and_metadata_to_SBOL2");
```

Methods to create annotations (String, URI, int, double, and nested).

```
String dcNS = "http://purl.org/dc/elements/1.1/";
genericTopLevel.createAnnotation(new QName(dcNS,"creator","dc"), "Prashant_Vaidyanathan");
genericTopLevel.createAnnotation(new QName(dcNS,"creator","dc"), "Chris_J._Myers");
TimeZone tz = TimeZone.getTimeZone("UTC");
DateFormat df = new SimpleDateFormat("yyyy-MM-dd'T'HH:mm'Z'");
df.setTimeZone(tz);
createdDate = df.format(new Date());
genericTopLevel.createAnnotation(new QName(provNS,"endedAtTime","prov"), createdDate);
```

GenericTopLevel (Example)

```
<rdf:RDF xmlns:rdf="http://www.w3.org/1999/02/22-rdf-syntax-ns#"</pre>
 xmlns:sbol="http://sbols.org/v2#"
 xmlns:dcterms="http://purl.org/dc/terms/"
 xmlns:prov="http://www.w3.org/ns/prov#"
 xmlns:dc="http://purl.org/dc/elements/1.1/">
 Activity rdf:about="http://cellocad.org/cello2sbol/1">
   <sbol:persistentIdentity rdf:resource="http://cellocad.org/cello2sbol"/>
   <sbol:displayId> cello2sbol</sbol:displayId>
   <sbol:version> 1</sbol:version>
   <dcterms:title> Cello UCF to SBOL conversion
   <dcterms:description> Conversion of the Cello UCF parts and metadata to SBOL2
   </dcterms:description>
   <dc:creator> Prashant Vaidyanathan</dc:creator>
   <dc:creator> Chris J. Myers</dc:creator>
   </rdf:RDF>
```

Cello UCF File

- JSON file format including the following sections:
 - Parts basic DNA parts (promoters, rbs, cds, terminators, etc.)
 - Gate parts compositions of DNA parts to form complete functions
 - Gates additional information about these gate parts
 - Other information response functions, gate toxicity, etc.

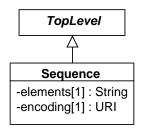
Cello UCF File Example

```
"collection": "parts",
  "type": "cds",
  "name": "AmtR".
  "dnasequence": "ATGGCAGGCGCAGTTGGTCGTCGCGTCGTAGTGCACCGCGTCGTGCAGGTAAAAATCCGCGTGAAGAAATTC..."
},...
  "collection": "gates".
  "regulator": "AmtR",
  "group name": "AmtR",
  "gate_name": "A1_AmtR",
  "gate type": "NOR",
  "system": "TetR",
  "color_hexcode": "3BA9E0"
  "collection": "gate_parts",
  "gate_name": "A1_AmtR",
  "expression cassettes": [
      "maps to variable": "x",
      "cassette parts": [
        "BydvJ",
        "A1",
        "AmtR".
        "L3S2P55"
  "promoter": "pAmtR"
}, ...
```

Parsing Cello JSON File

```
HashMap<String, JSONObject> partsMap = new HashMap<String, JSONObject>();
HashSet<JSONObject> gate partsArr = new HashSet<JSONObject>():
HashMap<String, JSONObject> gatesMap = new HashMap<String, JSONObject>();
JSONParser parser = new JSONParser();
JSONArray a = (JSONArray) parser.parse(new FileReader(JSONfilename));
for (Object o : a)
  JSONObject ucf = (JSONObject) o;
  String collection = (String) ucf.get("collection");
  if (collection.equals("parts")) {
    partsMap.put((String)ucf.get("name"),ucf);
  else if (collection.equals("gate_parts")) {
    gate partsArr.add(ucf);
  else if (collection.equals("gates"))
    gatesMap.put((String)ucf.get("gate name"),ucf);
```

Sequence¹



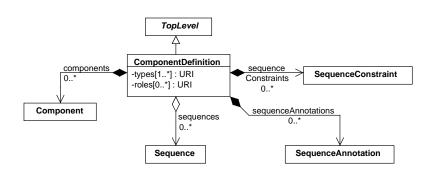
- elements String of characters representing constituents of a biological or chemical molecule.
- encoding URI indicating how elements are to be interpreted.

Encoding	URI	CD Type
IUPAC DNA, RNA	http://www.chem.qmul.ac.uk/iubmb/misc/naseq.html	DNA, RNA
IUPAC Protein	http://www.chem.qmul.ac.uk/iupac/AminoAcid/	Protein
SMILES	http://www.opensmiles.org/opensmiles.html	SmallMolecule

Creating Sequences for Parts

```
for (JSONObject part : partsMap.values()) {
 String name = (String)part.get("name");
 String dnasequence = (String)part.get("dnasequence");
 Sequence sequence = document.createSequence(name + " sequence", version, dnasequence,
   Sequence. IUPAC DNA);
 sequence.setName(name+" sequence");
 sequence.addWasDerivedFrom(derivedFrom);
 sequence.createAnnotation(new OName(provNS, "wasGeneratedBy", "prov"), activityURI);
 sequence.createAnnotation(new QName(dcTermsNS, "created", "dcTerms"), createdDate);
<sbol:Sequence rdf:about="http://cellocad.org/AmtR sequence/1">
 <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR sequence"/>
 <sbol:displayId> AmtR sequence </sbol:displayId>
 <sbol:version> 1 </sbol:version>
 <dcterms:title> AmtR sequence </dcterms:title>
 <dcterms:created> 2017-08-09T13:54Z </dcterms:created>
 <sbol:elements> ATGGCAGGCGCAGTTGGTCGTCGTCGTGGTGGTGCACCGCGTCGTGCAGGTAAAATCCGCGTGAAGAATTCTGGATGC
 <sbol:encoding rdf:resource="http://www.chem.gmul.ac.uk/iubmb/misc/naseg.html"/>
</sbol:Sequence>
```

ComponentDefinition



ComponentDefinition (Types/Roles)

CD Type	URI for BioPAX Term
DNA	http://www.biopax.org/release/biopax-level3.owl#DnaRegion
RNA	http://www.biopax.org/release/biopax-level3.owl#RnaRegion
Protein	http://www.biopax.org/release/biopax-level3.owl#Protein
Small Molecule	http://www.biopax.org/release/biopax-level3.owl#SmallMolecule
Complex	http://www.biopax.org/release/biopax-level3.owl#Complex

CD Role	URI for SequenceOntology Term	CD 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

Converting Part Type to SBOL ComponentDefinition Role

```
public static URI getRole(String type) {
String so = "http://identifiers.org/so/";
if (type.equals("ribozyme")) {
    return URI.create(so + "SO:0000374");
 else if (type.equals("scar")) {
    return URI.create(so + "SO:0001953");
 else if (type.equals("cds")) {
    return URI.create(so + "SO:0000316");
 else if (type.equals("promoter")) {
    return URI.create(so + "S0:0000167");
 else if (type.equals("rbs")) {
    return URI.create(so + "S0:0000139");
 else if (type.equals("terminator")) {
    return URI.create(so + "SO:0000141");
  } else {
    System.err.println("Part_Type_not_found");
   return null;
```

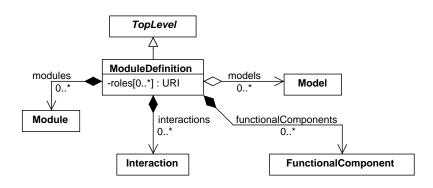
Converting Parts to SBOL ComponentDefinitions

```
ComponentDefinition componentDefinition =
  document.createComponentDefinition(name, version, ComponentDefinition.DNA);
 componentDefinition.setName(name);
 componentDefinition.addWasDerivedFrom(derivedFrom);
 componentDefinition.createAnnotation(new OName(provNS, "wasGeneratedBy", "prov"), activityURI);
 componentDefinition.createAnnotation(new QName(dcTermsNS, "created", "dcTerms"), createdDate);
 String partType = (String)part.get("type");
 componentDefinition.addRole(getRole(partType));
 componentDefinition.addSequence(sequence);
 if (partType.equals("cds")) {
   ComponentDefinition proteinComponentDefinition =
     document.createComponentDefinition(name+" protein", version, ComponentDefinition.PROTEIN);
   proteinComponentDefinition.setName(name+"_protein");
   proteinComponentDefinition.createAnnotation(new QName(provNS,"wasGeneratedBy","prov"),
     activityURI);
   proteinComponentDefinition.createAnnotation(new OName(dcTermsNS, "created", "dcTerms"),
     createdDate):
```

Converting Parts to SBOL ComponentDefinitions

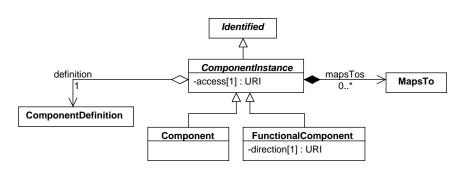
```
<sbol:ComponentDefinition rdf:about="http://cellocad.org/AmtR/1">
  <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR"/>
  <sbol:displayId> AmtR </sbol:displayId>
  <sbol:version> 1 </sbol:version>
  <prev:wasDerivedFrom rdf:resource="https://github.com/CIDARLAB/cello/blob/master/resources/UCF/E</pre>
  <dcterms:title> AmtR </dcterms:title>
  <dcterms:created> 2017-08-09T13:547 </dcterms:created>
  <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#DnaRegion"/>
  <sbol:role rdf:resource="http://identifiers.org/so/S0:0000316"/>
  <sbol:sequence rdf:resource="http://cellocad.org/AmtR sequence/1"/>
</sbol:ComponentDefinition>
<sbol:ComponentDefinition rdf:about="http://cellocad.org/AmtR protein/1">
  <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR protein"/>
  <sbol:displayId> AmtR protein </sbol:displayId>
  <sbol:version> 1 </sbol:version>
  <dcterms:title> AmtR protein </dcterms:title>
  <prev:wasGeneratedBy rdf:resource="http://cellocad.org/cello2sbol/1"/>
  <dcterms:created> 2017-08-09T13:547 </dcterms:created>
  <sbol:type rdf:resource="http://www.biopax.org/release/biopax-level3.owl#Protein"/>
</sbol:ComponentDefinition>
```

ModuleDefinition



Creating ModuleDefinitions for Genetic Production

FunctionalComponent (Child of ModuleDefinition)



Access URI

http://sbols.org/v2#public http://sbols.org/v2#private

Direction URI

http://sbols.org/v2#in http://sbols.org/v2#out http://sbols.org/v2#inout http://sbols.org/v2#none

Description

MAY be referred to by remote MapsTo objects.

MUST NOT be referred to by remote **MapsTo** objects.

Description

Indicates that it is an input.

Indicates that it is an output.

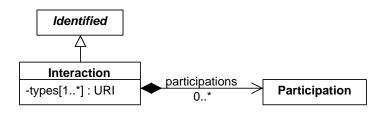
Indicates that it is both an input and output

Indicates that it is neither an input and output.

Creating FunctionalComponents for Genetic Production

```
moduleDefinition.createFunctionalComponent(name, AccessType.PUBLIC,
  componentDefinition.getIdentity(), DirectionType.NONE);
moduleDefinition.createFunctionalComponent(name+" protein", AccessType.PUBLIC,
  proteinComponentDefinition.getIdentity(), DirectionType.NONE);
<sbol:ModuleDefinition rdf:about="http://cellocad.org/AmtR protein production/1">
  <sbol:functionalComponent>
    <sbol:FunctionalComponent rdf:about="http://cellocad.org/AmtR protein production/AmtR/1">
      <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR_protein_production/AmtR"/>
      <sbol:displayId> AmtR </sbol:displayId>
      <sbol:version> 1 </sbol:version>
      <sbol:definition rdf:resource="http://cellocad.org/AmtR/1"/>
      <sbol:access rdf:resource="http://sbols.org/v2#public"/>
      <sbol:direction rdf:resource="http://sbols.org/v2#none"/>
    </sbol:FunctionalComponent>
  </sbol:functionalComponent>
  <sbol:functionalComponent>
    <sbol:FunctionalComponent rdf:about="http://cellocad.org/AmtR_protein_production/AmtR_protein/</pre>
      <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR protein production/AmtR prot</pre>
      <sbol:displayId> AmtR_protein </sbol:displayId>
      <sbol:version> 1 </sbol:version>
      <sbol:definition rdf:resource="http://cellocad.org/AmtR protein/1"/>
      <sbol:access rdf:resource="http://sbols.org/v2#public"/>
      <sbol:direction rdf:resource="http://sbols.org/v2#none"/>
    </sbol:FunctionalComponent>
  </sbol:functionalComponent>
</sbol:ModuleDefinition>
```

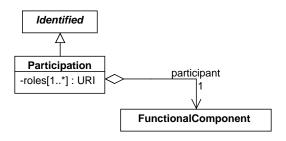
Interaction (Child of ModuleDefinition)



Interaction Type URI for SystemsBiologyOntology Term

National Systems biology of Na

Participation (Child of Interaction)



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

Interaction Types

Biochemical Reaction, Control

Biochemical Reaction, Control

Genetic Production

Chris J. Mvers (University of Utah)

LIRI for SRO Term

Part Role

Modifier

Modified

Template

http://identifiers.org/biomodels.sbo/SBO:0000019

http://identifiers.org/biomodels.sbo/SBO:0000644

http://identifiers.org/biomodels.sbo/SBO:0000645

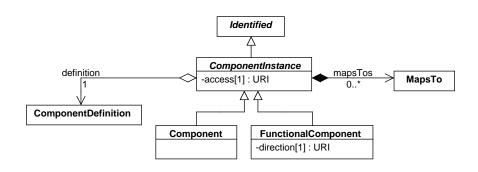
Creating Interactions for Genetic Production

```
Interaction interaction = moduleDefinition.createInteraction(name+" protein interaction",
  SystemsBiologyOntology.GENETIC PRODUCTION);
interaction.createParticipation(name, name, SystemsBiologyOntology.TEMPLATE);
interaction.createParticipation(name+" protein", name+" protein", SystemsBiologyOntology.PRODUCT);
  <sbol:interaction>
    <sbol:Interaction rdf:about="http://cellocad.org/AmtR protein production/AmtR protein interact</pre>
      <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR_protein_production/AmtR_prot</pre>
      <sbol:displayId> AmtR protein interaction </sbol:displayId>
      <sbol:version> 1 </sbol:version>
      <sbol:type rdf:resource="http://identifiers.org/biomodels.sbo/SB0:0000589"/>
      <sbol:participation>
        <sbol:Participation rdf:about="http://cellocad.org/AmtR protein production/AmtR protein in</pre>
          <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR protein production/AmtR</pre>
          <sbol:displayId> AmtR </sbol:displayId>
          <sbol:version> 1 </sbol:version>
          <sbol:role rdf:resource="http://identifiers.org/biomodels.sbo/SBO:0000645"/>
          <sbol:participant rdf:resource="http://cellocad.org/AmtR protein production/AmtR/1"/>
        </sbol:Participation>
      </sbol:participation>
      <sbol:participation>
        <sbol:Participation rdf:about="http://cellocad.org/AmtR protein production/AmtR protein in</pre>
          <sbol:persistentIdentity rdf:resource="http://cellocad.org/AmtR protein production/AmtR</pre>
          <sbol:displayId> AmtR_protein </sbol:displayId>
          <sbol:version> 1 </sbol:version>
          <sbol:role rdf:resource="http://identifiers.org/biomodels.sbo/SB0:0000011"/>
          <sbol:participant rdf:resource="http://cellocad.org/AmtR protein production/AmtR protein</pre>
        </sbol:Participation>
      </sbol:participation>
    </sbol:Interaction>
  </sbol:interaction>
</sbol:ModuleDefinition>
```

Converting Gate Parts to SBOL ComponentDefinitions

```
for (JSONObject gate : gate partsArr) {
 String gate name = (String)gate.get("gate name");
 ComponentDefinition componentDefinition =
   document.createComponentDefinition(gate name, version, ComponentDefinition.DNA);
 componentDefinition.setName(gate_name);
 componentDefinition.addRole(SequenceOntology.ENGINEERED REGION);
 componentDefinition.addWasDerivedFrom(derivedFrom);
 componentDefinition.createAnnotation(new QName(provNS,"wasGeneratedBy","prov"), activityURI);
 componentDefinition.createAnnotation(new OName(dcTermsNS, "created", "dcTerms"), createdDate);
 componentDefinition.createAnnotation(new OName(celloNS, "family", "cello"),
    (String) gatesMap.get(gate name).get("system"));
 componentDefinition.createAnnotation(new QName(celloNS, "gate type", "cello"),
    (String) gatesMap.get (gate_name).get ("gate_type"));
 componentDefinition.createAnnotation(new QName(celloNS, "group name", "cello"),
    (String) gatesMap.get(gate name).get("group name"));
 componentDefinition.createAnnotation(new OName(celloNS, "color hexcode", "cello"),
    (String) gatesMap.get(gate_name).get("color_hexcode"));
```

Component (Child of ComponentDefinition)



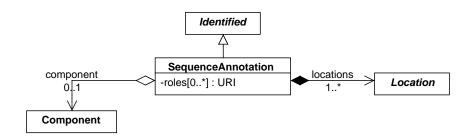
Access URI

http://sbols.org/v2#public http://sbols.org/v2#private

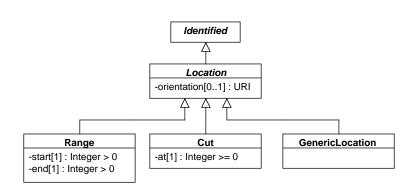
Description

MAY be referred to by remote **MapsTo** objects. MUST NOT be referred to by remote **MapsTo** objects.

SequenceAnnotation (Child of ComponentDefinition)



Location (Child of SequenceAnnotation)



Orientation URI

http://sbols.org/v2#inline http://sbols.org/v2#reverseComplement

Description

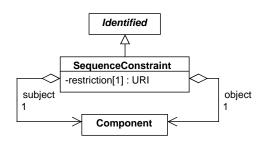
The region is inline with the sequence.

The region is on the reverse-complement translation.

Creating Composite Gates Using SequenceAnnotations

```
JSONArray expression_cassettes = (JSONArray) gate.get("expression_cassettes");
String seg = "";
for (Object obj : expression_cassettes) {
 int annotationCount = 0;
 int start = 1:
 JSONObject expression cassette = (JSONObject) obj;
 JSONArray cassette parts = (JSONArray)expression cassette.get("cassette parts");
 for (Object obj2 : cassette parts) {
    String partId = (String)obj2;
    ComponentDefinition partComponentDefinition =
     document.getComponentDefinition(partId, version);
    String cass_seg = document.getSequence(partId+"_sequence",version).getElements();
    seq += cass seq;
    componentDefinition.createComponent(partId, AccessType.PUBLIC, partId, version);
    SequenceAnnotation sa =
     componentDefinition.createSequenceAnnotation("annotation"+annotationCount,
     "range", start, start + cass_seq.length() - 1, OrientationType.INLINE);
    sa.setComponent(partId);
    start += cass_seq.length();
    annotationCount ++:
```

SequenceConstraint (Child of ComponentDefinition)



Restriction URI

http://sbols.org/v2#precedes http://sbols.org/v2#sameOrientationAs http://sbols.org/v2#oppositeOrientationAs

Description

subject MUST precede object Component. subject & object MUST have same orientation. subject & object MUST have opposite orientations.

Creating Composite Gates Using SequenceConstraints

```
JSONArray expression_cassettes = (JSONArray) gate.get("expression_cassettes");
for (Object obj : expression_cassettes) {
 int constraintCount = 0;
 Component previousComponent = null:
 Component currentComponent = null:
 JSONObject expression cassette = (JSONObject) obj;
 JSONArray cassette_parts = (JSONArray)expression_cassette.get("cassette_parts");
 for (Object obj2 : cassette parts) {
    String partId = (String)obj2;
    ComponentDefinition partComponentDefinition =
     document.getComponentDefinition(partId, version);
    currentComponent = componentDefinition.createComponent(partId, AccessType.PUBLIC,
     partId, version);
    if (previousComponent != null) {
     componentDefinition.createSequenceConstraint("constraint"+constraintCount,
        RestrictionType.PRECEDES,
        previousComponent.getIdentity(), currentComponent.getIdentity());
     constraintCount ++:
    previousComponent = currentComponent;
```

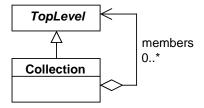
Creating ModuleDefinitions for Inhibition

```
if (partComponentDefinition.getRoles().contains(SequenceOntology.CDS)) {
  String promoter = (String)gate.get("promoter");
  if (document.getModuleDefinition(partId+"_"+promoter+"_repression", version) == null) {
    ModuleDefinition moduleDefinition =
      document.createModuleDefinition(partId+"_"+promoter+"_repression", version);
    moduleDefinition.createAnnotation(new OName(provNS, "wasGeneratedBy", "prov"), activityURI);
    moduleDefinition.createAnnotation(new OName(dcTermsNS, "created", "dcTerms"), createdDate);
    Interaction interaction =
      moduleDefinition.createInteraction(partId+" "+promoter+" repression",
      SystemsBiologyOntology.INHIBITION);
    interaction.createParticipation(partId+"_protein_participation", partId+"_protein",
      SystemsBiologyOntology.INHIBITOR);
    interaction.createParticipation(promoter+"_promoter_participation", promoter,
      SystemsBiologyOntology.INHIBITED):
```

Creating the Composite Sequence

```
Sequence sequence = document.createSequence(gate_name+"_sequence", version, seq,
    Sequence.IUPAC_DNA);
sequence.setName(gate_name+"_sequence");
sequence.addWasDerivedFrom(derivedFrom);
sequence.createAnnotation(new QName(provNS, "wasGeneratedBy", "prov"), activityURI);
sequence.createAnnotation(new QName(dcTermsNS, "created", "dcTerms"), createdDate);
componentDefinition.addSequence(sequence);
```

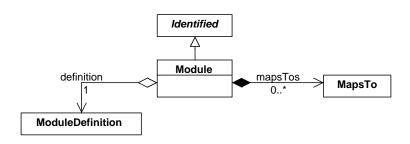
Collection



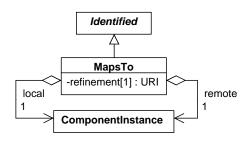
Creating CDS Part Collection

```
Collection cdsCollection = document.createCollection("cdsCollection", version);
for (ComponentDefinition cd : document.getComponentDefinitions()) {
  if (cd.containsRole(SequenceOntology.CDS)) {
    cdsCollection.addMember(cd.getIdentity());
<sbol:Collection rdf:about="http://cellocad.org/cdsCollection/1">
  <sbol:persistentIdentity rdf:resource="http://cellocad.org/cdsCollection"/>
  <sbol:displayId> cdsCollection </sbol:displayId>
  <sbol:version> 1 </sbol:version>
  <sbol:member rdf:resource="http://cellocad.org/SrpR/1"/>
  <sbol:member rdf:resource="http://cellocad.org/AmeR/1"/>
  <sbol:member rdf:resource="http://cellocad.org/HlvIIR/1"/>
  <sbol:member rdf:resource="http://cellocad.org/AmtR/1"/>
  <sbol:member rdf:resource="http://cellocad.org/PhlF/1"/>
  <sbol:member rdf:resource="http://cellocad.org/BM3R1/1"/>
  <sbol:member rdf:resource="http://cellocad.org/BetI/1"/>
</shol:Collection>
```

Module (Child of ModuleDefinition)



MapsTo (Child of ComponentInstance)



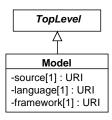
Refinement URI

http://sbols.org/v2#useRemote http://sbols.org/v2#useLocal http://sbols.org/v2#verifyIdentical http://sbols.org/v2#merge

Description

All references MUST dereference to the *remote* CI.
All references MUST dereference to the *local* CI.
The *definition* of the *local* and *remote* MUST be same CD.
All references MUST dereference to both objects.

Model



- source URI reference to the source file for the model.
- language URI that species language in which the model is implemented.
 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

• framework - URI that species modeling framework used.

Framework URI for SBO Term

Continuous http://identifiers.org/biomodels.sbo/SBO:0000062
Discrete http://identifiers.org/biomodels.sbo/SBO:0000063

Serialization Methods

SBOLWriter class:

```
SBOLWriter.setKeepGoing(true);
SBOLWriter.write(document, String OR File OR OutputStream);
SBOLWriter.write(document, String OR File OR OutputStream, fileType);
fileType = SBOLDocument.RDF, RDFV1, GEMBANK, FASTAformat
document.write(String OR File OR OutputStream, fileType);
SBOLWriter.clearErrors();
SBOLWriter.getNumErrors();
SBOLWriter.getErrors();
```

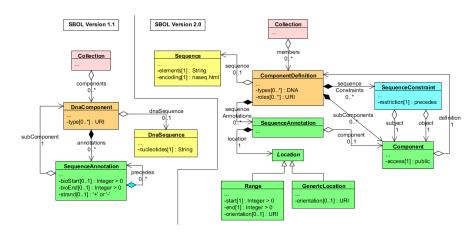
SBOLReader class:

```
SBOLReader.setURIPrefix("http://cellocad.org/");
SBOLReader.setVersion("!");
SBOLReader.setKeepGoing(true);

SBOLReader.getSBOLVersion(String OR File OR InputStream);
SBOLDocument document = SBOLReader.read(String OR File OR InputStream);
document.read(String OR File OR InputStream);
SBOLReader.clearErrors();
SBOLReader.getErrors();
SBOLReader.getErrors();
```

Conversion

- Supports conversion to/from GenBank and FASTA formats.
- Reads/Writes SBOL 1.1 data files.



Validation

Many validation rules checked when documents are read.

```
SBOLReader.setKeepGoing(true);
SBOLDocument document = SBOLReader.read(file);
if (SBOLReader.getNumErrors() > 0) {
    for(String error : SBOLReader.getErrors()) {
        System.out.println(error);
    }
}
```

• Remaining validation rules checked by validateSBOL method.

Method to compare to SBOLDocuments.

```
SBOLValidate.compareDocuments (file, document, file2, document2);
```

SynBioHub Repository Support

Uploading SBOL to SynBioHub:

Other SynBioHub functions:

More Information

- libSBOLj is open source under the Apache 2.0 License.
- More information:

http://sbolstandard.org/software/libSBOL/java/.

- Current snapshot on GitHub.
- Latest release (Version 2.1.0) and GitHub and Maven.
- Issue tracker for reporting bugs and feature requests.
- JavaDocs for all public methods.
- A brief getting started tutorial.
- A detailed code example and sample project for a CRISPR circuit.
- Several example code files.

sboljs - Javascript SBOL library

- Developed by James McLaughlin at Newcastle University and myself.
- Prerequisites: node.js and npm.
- Install: npm install sboljs

Creating an SBOL Document

```
var SBOLDocument = require('sboljs');
...
var sbol = new SBOLDocument();
```

Creating a GenericTopLevel

```
var actVersion = 1;
var actDisplayId = 'cello2sbol';
var actPersistantIdentity = urlprefix + actDisplayId;
var activityURI = actPersistantIdentity + '/' + actVersion;

const activity = sbol.genericTopLevel(activityURI, provNS + 'Activity');
activity.version = actVersion;
activity displayId = actDisplayId;
activity.name = 'Cello UCF to SBOL conversion';
activity.description = 'Conversion of the Cello UCF parts and metadata to SBOL2';
activity.addStringAnnotation(dcNS + 'creator', 'Prashant Vaidyanathan');
activity.addStringAnnotation(dcNS + 'creator', 'Chris J. Myers');
// TODO: Need to change to PROV endedAtTime
activity.addStringAnnotation('http://purl.org/dc/terms/created', today.toISOString() + '');
activity.persistentIdentity = actPersistantIdentity;
activity.uri = activityURI;
```

Parsing Cello UCF JSON File

```
var ucf = JSON.parse(fs.readFileSync(ucfFilepath) + '');
var gate partsArr = [];
var partsMap = {};
var partsSBOL = {}
var gatesMap = {};
//Go through the UCF file to store collections in local data structures (arrays and maps)
ucf.forEach(function (collection) {
    switch (collection.collection) {
        case 'parts':
            //partsArr.push(collection);
            partsMap[collection.name] = collection;
            break:
        case 'gate parts':
            gate_partsArr.push(collection);
            break:
       case 'gates':
            gatesMap[collection.gate name] = collection;
            break:
}, this);
```

Converting Parts to SBOL (1)

```
Object.keys(partsMap).forEach(function (partkey) {
    var part = partsMap[partkey];
    var partName = part.name;
    if (!(partName in partsSBOL)) {
        const componentDefinition = sbol.componentDefinition()
        componentDefinition.version = version;
        componentDefinition.displayId = part.name;
        componentDefinition.name = part.name;
        componentDefinition.persistentIdentity = urlprefix + componentDefinition.displayId;
        componentDefinition.uri = componentDefinition.persistentIdentity + '/' +
          componentDefinition.version;
        componentDefinition.wasDerivedFrom = derivedFrom;
        componentDefinition.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
        componentDefinition.addRole(getPartType(part.type));
        componentDefinition.addType(SBOLDocument.terms.dnaRegion);
        const sequence = sbol.sequence()
        sequence.displayId = part.name + ' sequence';
        sequence.name = part.name + '_sequence';
        sequence.version = version;
        sequence.elements = part.dnasequence;
        sequence.persistentIdentity = urlprefix + sequence.displayId;
        sequence.uri = sequence.persistentIdentity + '/' + sequence.version;
        sequence.wasDerivedFrom = derivedFrom;
        sequence.encoding = SBOLDocument.terms.dnaSequence;
        sequence.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
        componentDefinition.addSequence(sequence)
```

Converting Parts to SBOL (2)

```
// Create a Protein
if (part.type === 'cds') {
  const proteinComponentDefinition = sbol.componentDefinition();
  proteinComponentDefinition.version = version;
  proteinComponentDefinition.displayId = componentDefinition.displayId + ' protein';
  proteinComponentDefinition.name = componentDefinition.displayId + ' protein':
  proteinComponentDefinition.persistentIdentity = urlprefix +
    proteinComponentDefinition.displayId;
  proteinComponentDefinition.uri = proteinComponentDefinition.persistentIdentity + '/' +
    proteinComponentDefinition.version;
  proteinComponentDefinition.addType(SBOLDocument.terms.protein);
  proteinComponentDefinition.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
  partsSBOL[partName + '_protein'] = proteinComponentDefinition.uri;
  const moduleDefinition = sbol.moduleDefinition();
  moduleDefinition.name = proteinComponentDefinition.displayId + ' production';
  moduleDefinition.version = version;
  moduleDefinition.displayId = proteinComponentDefinition.displayId + ' production';
  moduleDefinition.persistentIdentity = urlprefix + moduleDefinition.displayId;
  moduleDefinition.uri = moduleDefinition.persistentIdentity + '/' + moduleDefinition.version;
  moduleDefinition.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
```

Converting Parts to SBOL (4)

```
//Functional Component for Coding sequence
const functionalComponentCDS = sbol.functionalComponent();
functionalComponentCDS.version = version;
functionalComponentCDS.displayId = componentDefinition.displayId + '_functionalComponent';
functionalComponentCDS.name = componentDefinition.name + ' functionalComponent';
functionalComponentCDS.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
  functionalComponentCDS.displayId;
functionalComponentCDS.uri = functionalComponentCDS.persistentIdentity + '/' +
  functionalComponentCDS.version;
functionalComponentCDS.definition = componentDefinition;
//Functional Component for Protein
const functionalComponentProt = sbol.functionalComponent();
functionalComponentProt.version = version;
functionalComponentProt.displayId = proteinComponentDefinition.displayId + ' functionalComponent';
functionalComponentProt.name = proteinComponentDefinition.name + ' functionalComponent';
functionalComponentProt.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
  functionalComponentProt.displayId;
functionalComponentProt.uri = functionalComponentProt.persistentIdentity + '/' +
  functionalComponentProt.version;
functionalComponentProt.definition = proteinComponentDefinition;
```

Converting Parts to SBOL (5)

```
//CDS to Protein interaction
const interaction = sbol.interaction();
interaction.displayId = proteinComponentDefinition.displayId + ' interaction';
interaction.name = interaction.displayId;
interaction.version = version;
interaction.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
 interaction.displayId;
interaction.uri = interaction.persistentIdentity + '/' + interaction.version;
interaction.addType(productionSBO);
const participationCDS = sbol.participation();
participationCDS.version = version;
participationCDS.name = componentDefinition.displayId + ' participation';
participationCDS.displayId = componentDefinition.displayId + ' participation';
participationCDS.persistentIdentity = interaction.persistentIdentity + '/' +
  participationCDS.displayId;
participationCDS.uri = participationCDS.persistentIdentity + '/' + participationCDS.version;
participationCDS.addRole(templateSBO);
participationCDS.participant = functionalComponentCDS;
const participationProt = sbol.participation();
participationProt.version = version;
participationProt.name = proteinComponentDefinition.displayId + ' participation';
participationProt.displayId = proteinComponentDefinition.displayId + '_participation';
participationProt.persistentIdentity = interaction.persistentIdentity + '/' +
  participationProt.displayId;
participationProt.uri = participationProt.persistentIdentity + '/' + participationProt.version;
participationProt.addRole(productSBO);
participationProt.participant = functionalComponentProt;
interaction.addParticipation(participationCDS);
interaction.addParticipation(participationProt);
```

Converting Parts to SBOL (6)

```
moduleDefinition.addFunctionalComponent(functionalComponentCDS);
    moduleDefinition.addFunctionalComponent(functionalComponentProt);
    moduleDefinition.addInteraction(interaction);
}
componentDefinition.addStringAnnotation('http://purl.org/dc/terms/created',
    datecreated.toISOString() + '');
    var uriVal = componentDefinition.uri;
    partsSBOL[partName] = uriVal;
}
}, this);
```

Converting Gate Parts to SBOL (1)

```
gate_partsArr.forEach(function (gpart) {
    var gpartName = gpart.gate_name;
    const componentDefinition = sbol.componentDefinition();
    componentDefinition.version = version;
    componentDefinition.displayId = gpartName;
    componentDefinition.name = gpartName;
    componentDefinition.persistentIdentity = urlprefix + componentDefinition.displayId;
    componentDefinition.uri = componentDefinition.persistentIdentity + '/' +
        componentDefinition.version;
    componentDefinition.wasDerivedFrom = derivedFrom;
    componentDefinition.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
    componentDefinition.addUriAnnotation(tetR_family, gatesMap[gpartName].system);
    componentDefinition.addUriAnnotation(group_name, gatesMap[gpartName].group_name);
    componentDefinition.addUriAnnotation(gate_type, gatesMap[gpartName].gate_type);
    componentDefinition.addUriAnnotation(color_hexcode, gatesMap[gpartName].color_hexcode);
```

Converting Gate Parts to SBOL (2)

```
gpart.expression_cassettes.forEach(function (expression_cassettesArr) {
  var seq = "";
  var annotationCount = 0;
  var start = 1;

  expression_cassettesArr.cassette_parts.forEach(function (cassette) {
    const component = sbol.component();
    component.version = version;
    component.displayId = cassette;
    component.name = cassette;
    component.persistentIdentity = componentDefinition.persistentIdentity + '/' +
    component.uri = component.persistentIdentity + '/' + component.version;
    component.definition = sbol.lookupURI(partsSBOI[cassette]);
    componentDefinition.addComponent(component);
```

Converting Gate Parts to SBOL (3)

```
var cass seg = partsMap[cassette].dnasequence;
  seq += cass seq;
  const sa = sbol.sequenceAnnotation();
  sa.displayId = 'annotation' + annotationCount;
  annotationCount++:
  sa.name = cassette;
  sa.version = version;
  sa.persistentIdentity = componentDefinition.persistentIdentity + '/' + sa.displayId;
  sa.uri = sa.persistentIdentity + '/' + sa.version;
  sa.component = component;
  sa.description = partsMap[cassette].type;
  const range = sbol.range();
  range.displayId = 'range';
  range.persistentIdentity = sa.persistentIdentity + '/' + range.displayId;
  range.version = version;
  range.uri = range.persistentIdentity + '/' + range.version;
  range.start = start;
  var end = start + cass seg.length - 1;
  range.end = end;
  range.orientation = 'http://sbols.org/v2#inline';
  sa.addLocation(range);
  componentDefinition.addSequenceAnnotation(sa);
```

Converting Gate Parts to SBOL (4)

```
//Create Protein - Promoter repression Module definition
if (partsMap[cassette].type === 'cds') {
  if (!(cassette in moduleDefnMap)) {
     const moduleDefinition = sbol.moduleDefinition();
      moduleDefinition.version = version;
      moduleDefinition.name = cassette + ' ' + gpart.promoter + ' repression';
      moduleDefinition.displayId = cassette + '_' + gpart.promoter + '_repression';
      moduleDefinition.persistentIdentity = urlprefix + moduleDefinition.displayId;
      moduleDefinition.uri = moduleDefinition.persistentIdentity + '/' +
        moduleDefinition.version:
      moduleDefinition.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
      const functionalComponentCDS = sbol.functionalComponent();
      functionalComponentCDS.version = version;
      functionalComponentCDS.name = cassette + '_protein_functionalComponent';
      functionalComponentCDS.displayId = cassette + '_protein_functionalComponent';
      functionalComponentCDS.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
        functionalComponentCDS.displayId;
      functionalComponentCDS.uri = functionalComponentCDS.persistentIdentity + '/' +
        functionalComponentCDS.version;
      functionalComponentCDS.definition = sbol.lookupURI(partsSBOL[cassette + ' protein'l);
      const functionalComponentProm = sbol.functionalComponent();
      functionalComponentProm.version = version;
      functionalComponentProm.name = gpart.promoter + '_functionalComponent';
      functionalComponentProm.displayId = gpart.promoter + ' functionalComponent';
      functionalComponentProm.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
        functionalComponentProm.displayId;
      functionalComponentProm.uri = functionalComponentProm.persistentIdentity + '/' +
        functionalComponentProm.version;
      functionalComponentProm.definition = sbol.lookupURI(partsSBOL[gpart.promoter]);
```

Converting Gate Parts to SBOL (5)

```
//Protein - Promoter Interaction
const interaction = sbol.interaction();
interaction.version = version;
interaction.name = cassette + '_' + qpart.promoter + '_interaction';
interaction.displayId = cassette + '_' + qpart.promoter + '_interaction';
interaction.persistentIdentity = moduleDefinition.persistentIdentity + '/' +
 interaction.displayId:
interaction.uri = interaction.persistentIdentity + '/' + interaction.version;
interaction.addType(inhibitionSO);
//Protein participation
const participantProt = sbol.participation();
participantProt.version = version;
participantProt.name = cassette + '_protein_participation';
participantProt.displayId = cassette + '_protein_participation';
participantProt.persistentIdentity = interaction.persistentIdentity + '/' +
  participantProt.displayId;
participantProt.uri = participantProt.persistentIdentity + '/' + participantProt.version;
participantProt.addRole(inhibitorSO);
participantProt.participant = functionalComponentCDS;
//Promoter participation
const participantProm = sbol.participation();
participantProm.version = version;
participantProm.name = gpart.promoter + '_participation';
participantProm.displayId = gpart.promoter + ' participation';
participantProm.persistentIdentity = interaction.persistentIdentity + '/' +
  participantProm.displayId;
participantProm.uri = participantProm.persistentIdentity + '/' + participantProm.version;
participantProm.addRole(inhibitedSO);
participantProm.participant = functionalComponentProm;
```

Converting Gate Parts to SBOL (6)

```
interaction.addParticipation(participantProt);
interaction.addParticipation(participantProm);

moduleDefinition.addFunctionalComponent(functionalComponentCDS);
moduleDefinition.addFunctionalComponent(functionalComponentProm);
moduleDefinition.addInteraction(interaction);

moduleDefnMap[cassette] = gpart.promoter;
}
start += cass_seq.length;
});
```

Converting Gate Parts to SBOL (7)

```
const sequence = sbol.sequence()
    sequence.displayId = gpartName + ' sequence';
    sequence.name = gpartName + '_sequence';
    sequence.version = version;
    sequence.elements = seq;
    sequence.persistentIdentity = urlprefix + sequence.displayId;
    sequence.uri = sequence.persistentIdentity + '/' + sequence.version;
    sequence.wasDerivedFrom = derivedFrom;
    sequence, encoding = SBOLDocument, terms, dnaSequence;
    sequence.addUriAnnotation(provNS + 'wasGeneratedBy', activityURI);
    componentDefinition.addSequence(sequence);
 }, this);
 componentDefinition.addType(SBOLDocument.terms.dnaRegion);
 componentDefinition.addRole(gate_parts_so);
 componentDefinition.addStringAnnotation('http://purl.org/dc/terms/created', datecreated.toISOStr
}, this);
```

Writing the SBOL File

```
var fs = require('fs');
fs.writeFile(resultSBOL, sbol.serializeXML(), function (err) {
    if (err) {
        return console.log(err);
    }
    console.log("Cello_SBOL_file_created!");
});
```

Conclusion (SBOL Compliant Software)

- Can either support all classes or only its structural subset.
- Can support import of SBOL, export of SBOL, or both (lossy/lossless).
- SBOL Test Suite is currently under development here: https://github.com/SynBioDex/SBOLTestSuite
- Validate SBOL files generated using the SBOL Validator found here: http://www.async.ece.utah.edu/sbol-validator/
- Report SBOL-compliant software to the SBOL editors (editors@sbolstandard.org), so it can be listed on the SBOL website.