libSBOLj 2.0: A Java Library to Support SBOL 2.0

Zhen Zhang[1], Tramy Nguyen[1], Meher Samineni[1], Nicholas Roehner[2], Goksel Misirli[3], Matthew Pocock[3], Ernst Oberortner[4], Jacob Beal[5], Kevin Clancy[6], Anil Wipat[3], Chris Myers[1]

[1]University of Utah
[2]Boston University
[3]Newcastle University
[4]DOE Joint Genome Institute
[5]Raytheon BBN Technologies
[6]ThermoFisher Scientific

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libSBOLj

- Crucial to the success of a standard is software infrastructure to support developers' integration of the standard within their tools.
- `libSBOLj` is a native Java implementation of the SBOL data structure, which provides an *application programmers interface* (API) for tool developers to interact with SBOL data objects.
- In addition, the library distribution includes detailed documentation for the class definitions and the methods provided by the API.
- Leveraging `libSBOLj` many software tools now support SBOL 1.1.
- `libSBOLj 2.0` will ease the adoption of SBOL 2.0 by tool developers.

SBOL 2.0 Data Model

- `libSBOLj 2.0` organizes all SBOL data within an *SBOL document*.
- Includes a list of each type of *top level* object: *collections*, *modules*, *components*, *sequences*, *models*, and *generic top level* objects.
- These lists are organized as hash maps to allow for easy search by their *unique reference identifiers* (URIs) and validation that they are distinct.
- Library includes methods for creating, updating, accessing, and removing these data objects, as well as, their child objects.

Creating an SBOLDocument

```
String prURI = "http://partsregistry.org";
SBOLDocument document = new SBOLDocument();
document.setDefaultURIprefix(prURI);
document.setComplete(true);
document.setCompliant(true);
document.setCreateDefaults(true);
document.setTypesInURIs(false);
```

- Default URI prefix - prefix to use when none provided to create method.
- Complete - ensure that all URI references point to valid SBOL objects.
- Compliant - ensure that all URIs in the document are compliant.
- Create defaults - implicitly create ComponentInstances as needed.
- Types in URIs - insert type in URIs between prefix and displayId.

Creating SBOL Data Objects

- SBOLDocument class includes create methods for each TopLevel object.
    - displayId 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.

$$\text{create}\langle\text{TopLevel}\rangle(\text{URIprefix, displayId, version, }\langle\text{required fields}\rangle)$$

```
ComponentDefinition TetR_promoter =
  document.createComponentDefinition("BBa_R0040", ComponentDefinition.DNA);
Sequence seq_187 = document.createSequence("seq_187",
  "tccctatcagtgatagagattgacatccctatcagtgatagagatactgagcac", Sequence.IUPAC_DNA);
```

Setting and Editing Optional Fields

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

```
TetR_promoter.setName("p_tetR");
TetR_promoter.setDescription("TetR␣repressible␣promoter");
if (TetR_promoter.isSetName()) {
  TetR_promoter.unsetName();
  TetR_promoter.setName("p(tetR)");
}
```

- Methods to add and remove URIs from lists, as well as to check if it contains a URI.

```
TetR_promoter.addRole(SequenceOntology.PROMOTER);
URI TetR_promoter_role2 = URI.create("http://identifiers.org/so/SO:0000613");
TetR_promoter.addRole(TetR_promoter_role2);
if (TetR_promoter.containsRole(TetR_promoter_role2)) {
  TetR_promoter.removeRole(TetR_promoter_role2);
}
```

- Methods to clear, get, and set lists of URIs.

```
TetR_promoter.clearRoles();
if (!TetR_promoter.getRoles().isEmpty()) {
  System.out.println("TetR_promoter␣set␣is␣not␣empty");
}
TetR_promoter.setRoles(new HashSet<URI>(Arrays.asList(SequenceOntology.PROMOTER)));
```

Creating and Editing References

- Methods to add referenced objects.

```
TetR_promoter.addSequence(seq_187);
TetR_promoter.addSequence(seq_187.getIdentity());
```

- Methods to check if referenced object in the list, remove it, clear or set the entire list.

```
if (TetR_promoter.containsSequence(seq_187.getIdentity())) {
  TetR_promoter.removeSequence(seq_187.getIdentity());
}
TetR_promoter.clearSequences();
TetR_Promoter.setSequence(new HashSet<URI>(Arrays.asList(seq_187.getIdentity())));
```

- Methods to get list of referenced objects (complete documents only) or list of referenced URIs.

```
for (Sequence sequence : TetR_promoter.getSequences());
for (URI sequenceURI : TetR_promoter.getSequenceURIs());
```

Creating and Editing Child Objects

- Child object create methods only require displayId as URIprefix and Version inferred from the parent object.
- All required fields are additional parameters.

```
pIKELeftCassette.createSequenceConstraint(
  "pIKELeftCassette_sc",
  RestrictionType.PRECEDES,
  TetR_promoter.getDisplayId(),
  LacI_repressor.getDisplayId()
);
```

Copying/Renaming TopLevel Objects

- Four variants of createCopy and rename methods.

```
createCopy(topLevel);  // creates identical copy (must be into new document)
createCopy(topLevel, displayId);          // copy with new displayId
createCopy(topLevel, displayId, version); // copy with new displayId/version
createCopy(topLevel, URIprefix, displayId, version);
                                // copy with new URIprefix/displayId/version

ComponentDefinition TetR_promoter_copy =
  (ComponentDefinition)document.createCopy(TetR_promoter , "BBa_K137046");
ComponentDefinition TetR_promoter_rename =
  (ComponentDefinition)document.rename(TetR_promoter , "BBa_K137046");
```

- Copy TopLevel object and all objects that it references into a new SBOLDocument.

```
SBOLDocument newDoc = document.createRecursiveCopy(TetR_promoter);
```

Ontology Support

- Built-in support for several ontologies:
  - Sequence Ontology (SO) - for DNA type ComponentDefinition roles.
  - SystemsBiologyOntology (SBO) - for Model frameworks, Interaction types and Participation roles.
  - EDAM - for Model languages.

```
SequenceOntology.PROMOTER // Constants for common terms
SequenceOntology sequenceOntology = new SequenceOntology();
if (sequenceOntology.isDescendantOf(SequenceOntology.TERMINATOR,
  SequenceOntology.SEQUENCE_FEATURE)) {
  // Terminator is a sequence feature
}
for (URI termURI : sequenceOntology.getDescendantURIsOf(SequenceOntology.TERMINATOR)) {
  System.out.println("Id␣=␣" + getId(termURI) + "␣Name␣=␣" + getName(termURI));
}
```

- Several similar methods with different parameters or return values.

Annotations and GenericTopLevel Objects

- Software tools that need to store data that is not currently encoded within SBOL can do so using generic top level objects and custom annotations.
- When the library reader encounters a tag for a top level object that it does not recognize, this data is stored within a generic top level object.
- Within top level 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 Annotations / GenericTopLevel Objects

- Methods to create Boolean, double, integer, String, URI, and nested annotations.

```
String prPrefix = "pr";
TetR_promoter.createAnnotation(new QName(prURI, "experience", prPrefix),
  URI.create("http://parts.igem.org/Part:BBa_R0040"));
```

- GenericTopLevel objects mostly composed of annotations.

```
String myersLabURI = "http://www.async.ece.utah.edu";
String myersLabPrefix = "myersLab";
GenericTopLevel datasheet=document.createGenericTopLevel("datasheet", "1.0",
  new QName(myersLabURI, "datasheet", myersLabPrefix));
datasheet.setName("Datasheet␣for␣Custom␣Parameters");
datasheet.createAnnotation(
  new QName(myersLabURI, "characterizationData", myersLabPrefix),
  URI.create(myersLabURI + "/measurement/Part:BBa_R0040"));
datasheet.createAnnotation(
  new QName(myersLabURI, "transcriptionRate", myersLabPrefix), 0.75);
TetR_promoter.createAnnotation(
  new QName(myersLabURI, "datasheet", myersLabPrefix),
  datasheet.getIdentity());
```

Serialization Methods

- SBOLReader class:

```
SBOLReader.setURIPrefix("http://www.myparts.org");
SBOLReader.setVersion("1.0");
SBOLReader.setTypesInURI(false);
SBOLReader.setCompliant(true);
SBOLReader.setDropObjectsWithDuplicateURIs(false);
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.getNumErrors();
SBOLReader.getErrors();
```

- SBOLWriter class:

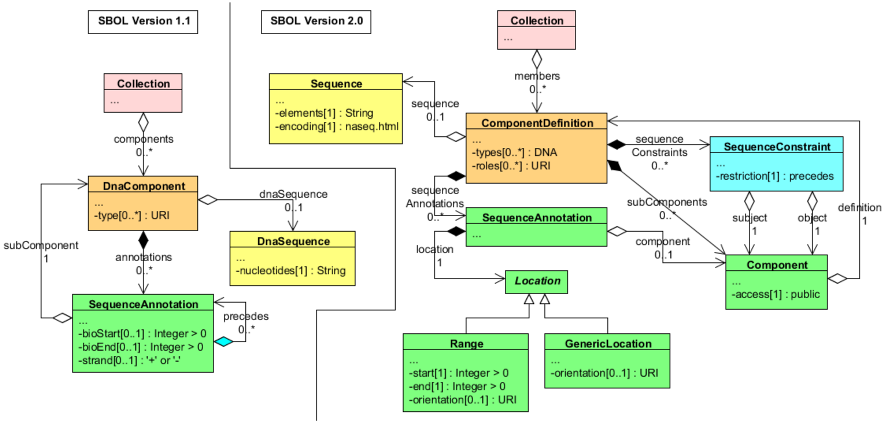
```
SBOLWriter.setKeepGoing(true);

SBOLWriter.write(document, String OR File OR OutputStream);
SBOLWriter.write(document, String OR File OR OutputStream, fileType);
fileType = SBOLDocument.RDF, RDFV1, GENBANK, FASTAformat
document.write(String OR File OR OutputStream, fileType);

SBOLWriter.clearErrors();
SBOLWriter.getNumErrors();
SBOLWriter.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.

```
boolean complete = true;     // Check that all referenced objects are included
boolean compliant = true;    // Check that all URIs are compliant
boolean bestPractice = true; // Check best practice validation rules
SBOLValidate.validateSBOL(document,complete,compliant,bestPractice);
if (SBOLValidate.getNumErrors() > 0) {
    for(String error : SBOLValidate.getErrors()) {
        System.out.println(error);
    }
}
```

- Method to compare to SBOLDocuments.

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

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 (basis for this talk).
    - A detailed code example and sample project for CRISPR circuit.
    - Several example code files.

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