libSBML & SBML

Sarah Keating

EMBL-EBI

EBI is an Outstation of the European Molecular Biology Laboratory.

SBML

A machine-readable format for representing computational models in systems biology

libSBML

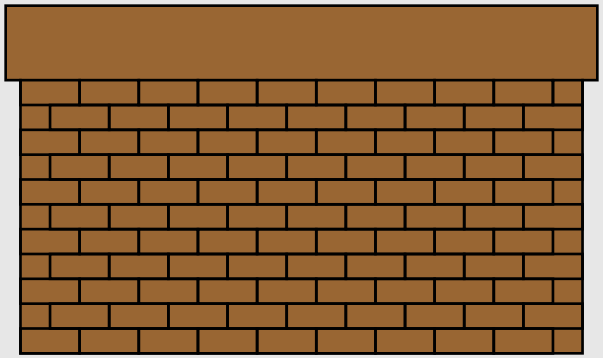
- API library for working with SBML

libSBML

- read

libSBML

- read
- create

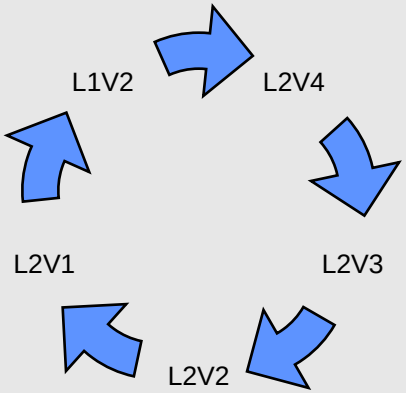


libSBML

- read
- create
- manipulate

libSBML

- read
- create
- manipulate
- convert between levels/versions



libSBML

- read
- create
- manipulate
- convert between levels/versions
- write

libSBML

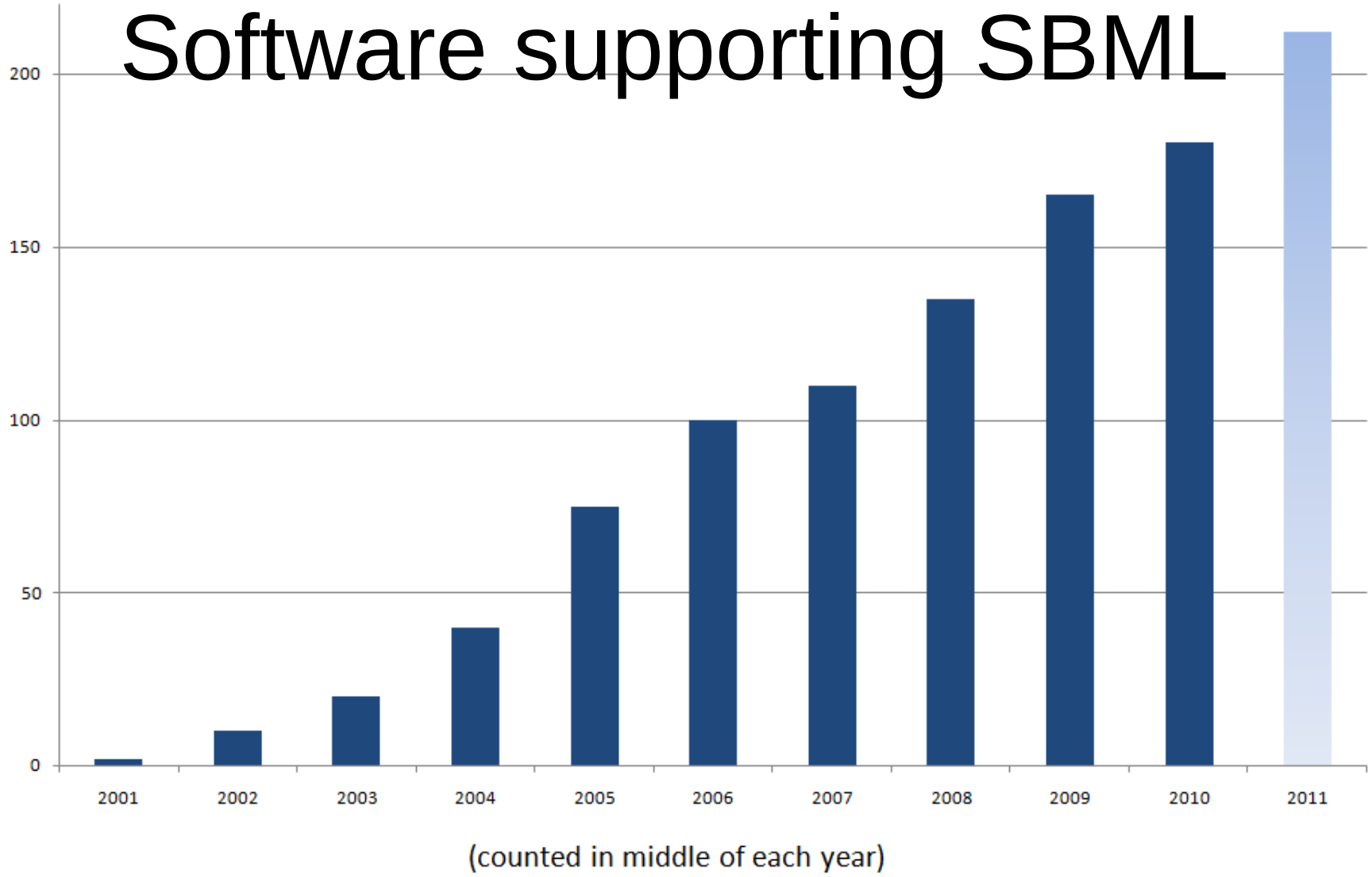
- read
- create
- manipulate
- convert between levels/versions
- write
- validate

libSBML

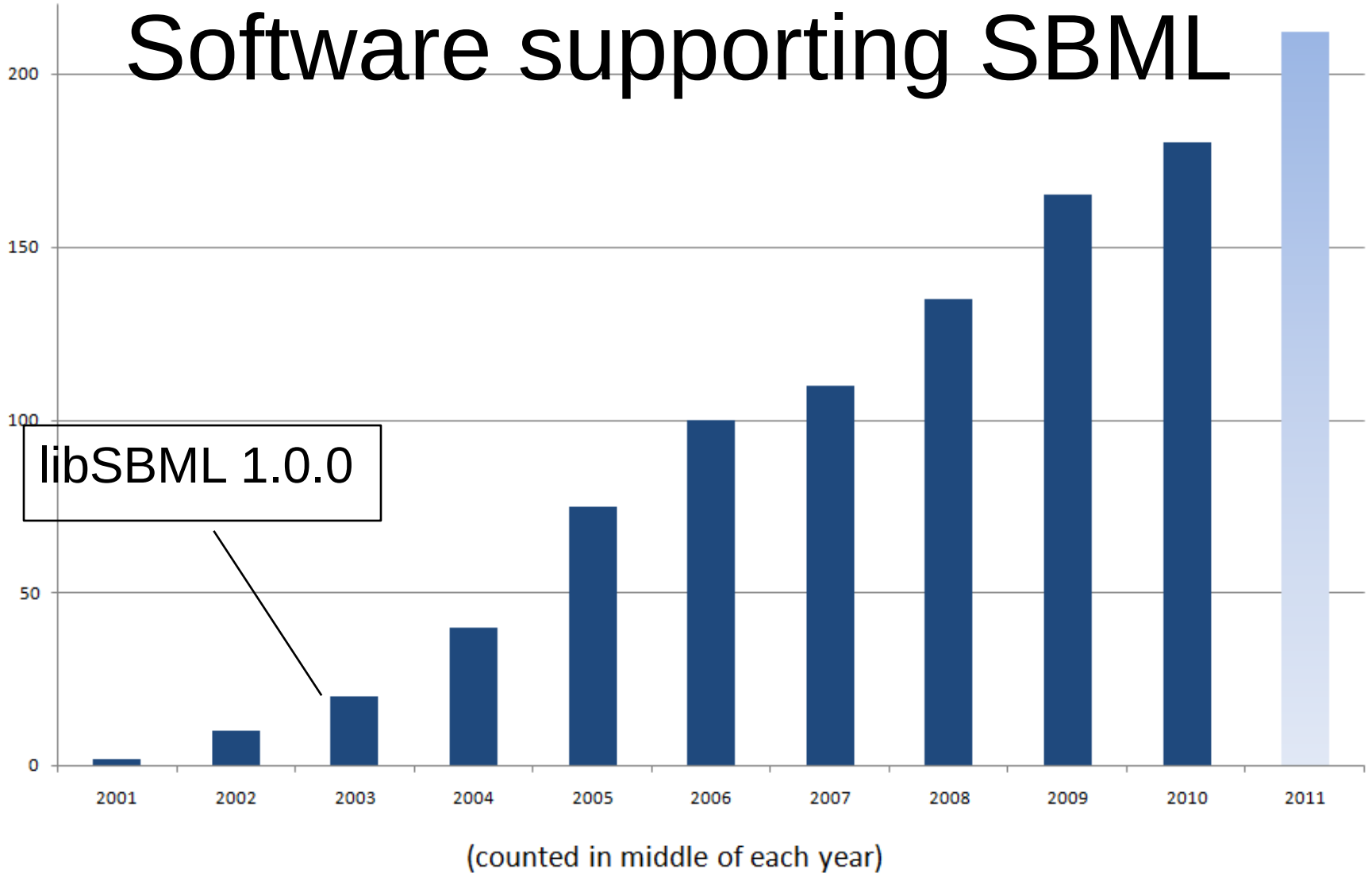
- API library for working with SBML

and the benefits to SBML

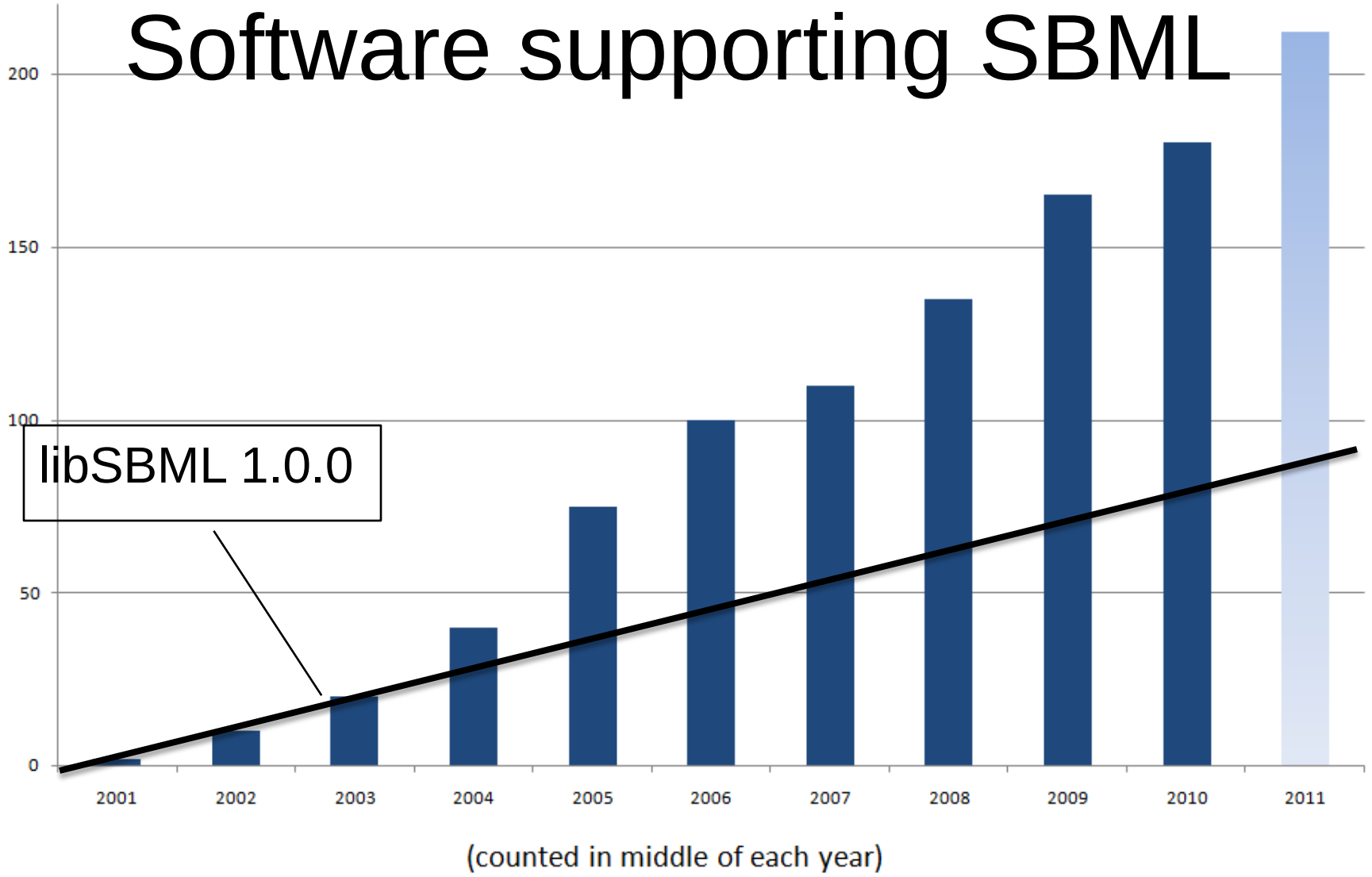
Software supporting SBML



Software supporting SBML



Software supporting SBML



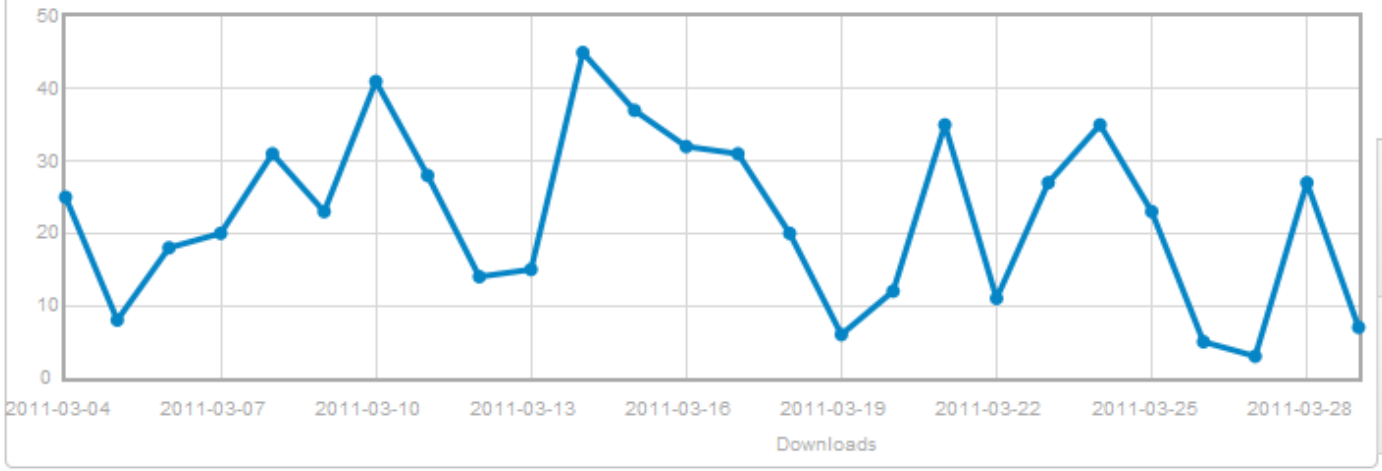
libSBML

Systems Biology Markup Language (SBML) by ajouraku, bbornstein, beshapiro, funa, luciansmith, mhucka, niko-rodrigue, sarahkeating

Summary | Files | Reviews | Support | Develop

Home / libsbml / 4.3.0 (Change File)

Date Range: 2011-03-04 to 2011-03-29



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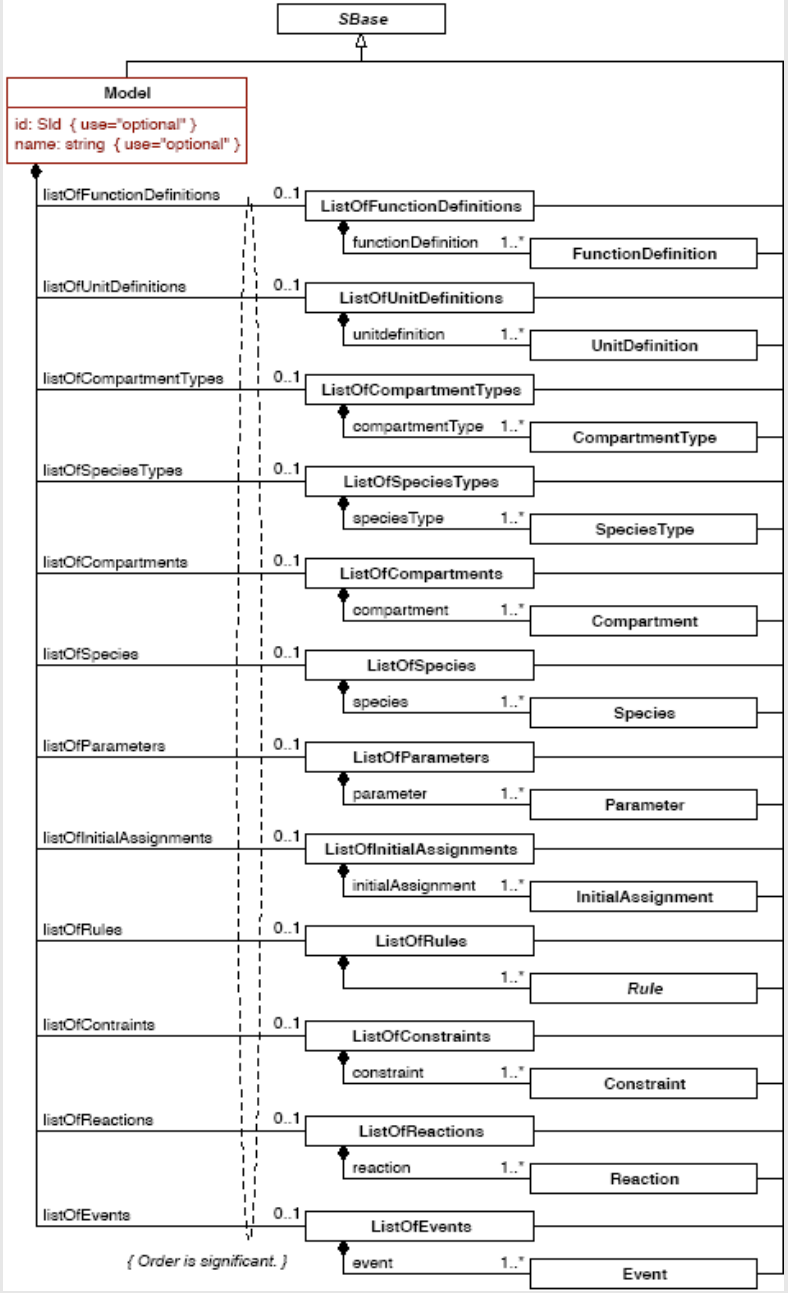
libSBML

- closely mimic SBML structure


SBase
Model
id: SId { use="optional" }
name: string { use="optional" }
listOfFunctionDefinitions
0..1
ListOfFunctionDefinitions
functionDefinition
1..*
FunctionDefinition
listOfUnitDefinitions
0..1
ListOfUnitDefinitions
unitdefinition
1..*
UnitDefinition
listOfCompartmentTypes
0..1
ListOfCompartmentTypes
compartmentType
1..*
CompartmentType
listOfSpeciesTypes
0..1
ListOfSpeciesTypes
speciesType
1..*
SpeciesType
listOfCompartments
0..1
ListOfCompartments
compartment
1..*
Compartment
listOfSpecies
0..1
ListOfSpecies
species
1..*
Species
listOfParameters
0..1
ListOfParameters
parameter
1..*
Parameter
listOfInitialAssignments
0..1
ListOfInitialAssignments
initialAssignment
1..*
InitialAssignment
listOfRules
0..1
ListOfRules
1..*
Rule
listOfContraints
0..1
ListOfConstraints
constraint
1..*
Constraint
listOfReactions
0..1
ListOfReactions
reaction
1..*
Reaction
listOfEvents
0..1
ListOfEvents
{ Order is significant. }
event
1..*
Event

Model.h

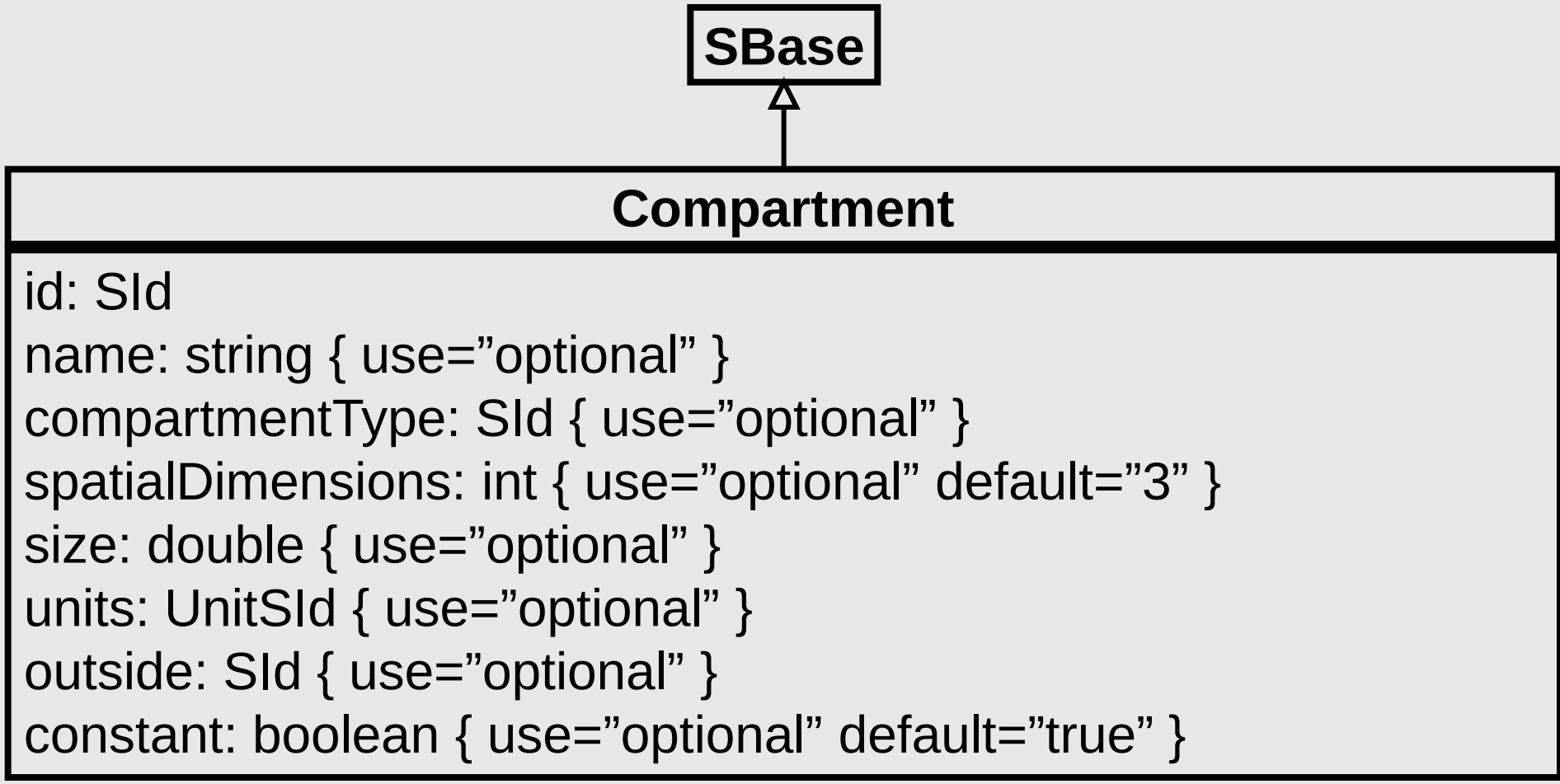
Model

```
  ModelHistory*   mHistory;


  ListOfFunctionDefinitions  mFunctionDefinitions;
  ListOfUnitDefinitions      mUnitDefinitions;
  ListOfCompartmentTypes     mCompartmentTypes;
  ListOfSpeciesTypes         mSpeciesTypes;
  ListOfCompartments         mCompartments;
  ListOfSpecies              mSpecies;
  ListOfParameters           mParameters;
  ListOfInitialAssignments   mInitialAssignments;
  ListOfRules                mRules;
  ListOfConstraints          mConstraints;
  ListOfReactions            mReactions;
  ListOfEvents               mEvents;

  ListFormulaUnitsData       mFormulaUnitsData;


#ifdef USE_LAYOUT
  ListOfLayouts mLayouts;
#endif  /* USE_LAYOUT */
```


SBase
Compartment
id: SId
name: string { use=”optional” }
compartmentType: SId { use=”optional” }
spatialDimensions: int { use=”optional” default=”3” }
size: double { use=”optional” }
units: UnitSId { use=”optional” }
outside: SId { use=”optional” }
constant: boolean { use=”optional” default=”true” }

File Edit View Project Build Debug Tools Window Help

Compartment.h

Compartment

Compartment

```
class LIBSBML_EXTERN Compartment : public SBase
{
  . . .

protected:
  /** @cond doxygen-libsbml-internal */


  /**
   * Subclasses should override this method to read values from the given
   * XMLAttributes set into their specific fields.  Be sure to call your
   * parents implementation of this method as well.
   */
  virtual void readAttributes (const XMLAttributes& attributes);


  /**
   * Subclasses should override this method to write their XML attributes
   * to the XMLOutputStream.  Be sure to call your parents implementation
   * of this method as well.
   */
  virtual void writeAttributes (XMLOutputStream& stream) const;


  std::string   mCompartmentType;
  unsigned int  mSpatialDimensions;
  double        mSize;
  std::string   mUnits;
  std::string   mOutside;
  bool          mConstant;

  bool  mIsSetSize;

  /** @endcond doxygen-libsbml-internal */
};
```

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```

libSBML

- closely mimic SBML structure
- different language bindings

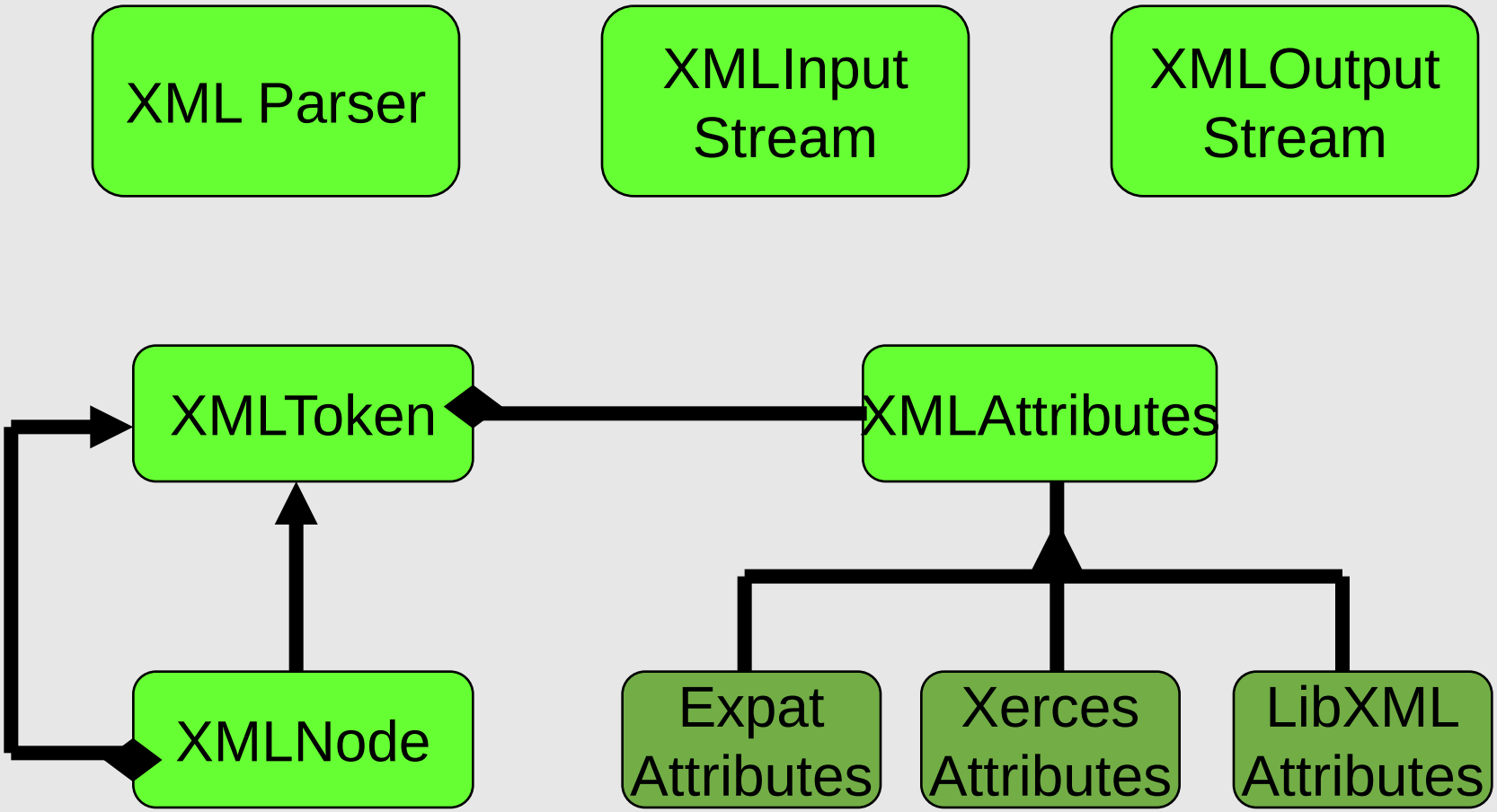
- Standard ANSI C++

- C
- C#
- Python
- MATLAB
- Java
- Octave
- Perl
- Ruby

libSBML

- closely mimic SBML structure
- different language bindings
- XML parsers

XML Layer


XML Parser
XMLInput Stream
XMLOutput Stream
XMLToken
XMLAttributes
XMLNode
Expat Attributes
Xerces Attributes
LibXML Attributes

libSBML

- closely mimic SBML structure
- different language bindings
- XML parsers
- develop in line with specification

libSBML

- closely mimic SBML structure
- different language bindings
- XML parsers
- develop in line with specification
- backwards compatibility

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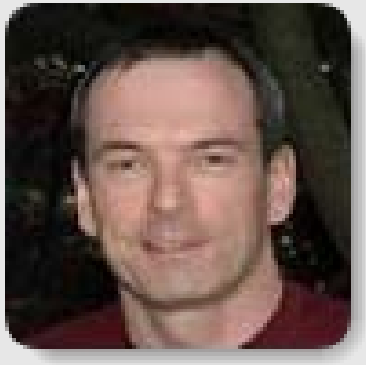

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