The function of this converter is to convert SBML files to the StochKit2 model definition format.

Installation

The converter uses the libSBML library.

If you already have libSBML version 4.1.0 or later installed, skip to the next section

Installing libSBML
- Navigate to the StochKit tools/SBMLconverter directory
- Unzip the libsbml distribution (unzip libsbml-4.1.0-b1-src.zip)
- cd into the directory libsbml-4.1.0-b1
- To specify an installation location, use
  ./configure --prefix="/my/favorite/path"
  otherwise the header files will be copied to /usr/local/include/sbml, the shared and static library files will be copied to /usr/local/lib. If you do not have administrator privileges, you will have to use the --prefix option.
- If your libxml2 is not installed in the standard location (e.g. a private home directory), you should explicitly tell the configure where to find the libraries. Use the command:
  ./configure --with-libxml="DIR"
  where DIR is the parent directory of the include and lib directories of libxml2.
- Type 'make'
- Type 'make install'
- If you specified an installation location, add environment variable (in Unix/Linux bash shell):
  export LD_LIBRARY_PATH="/my/favorite/path/lib:$LD_LIBRARY_PATH"
  for Mac OS X, replace LD_LIBRARY_PATH with DYLD_LIBRARY_PATH. To make the environment variable permanent, you should put the above line in a startup file, e.g. ~/.bashrc (instructions for setting environment variables can easily be found via your favorite search engine).

Compiling the StochKit2 SBML converter
- Navigate to the tools/SBMLconverter directory
- If libxml2 or libSBML are installed in a non-standard location, open the file named "Makefile" in a text editor
  - Edit the paths after "LIBSBML_PATH", "LIBXML_PATH", and "LINK_SEARCH_PATH" as necessary

    e.g.

    LIBSBML_PATH=/my/favorite/path/include

    and

    LINK_SEARCH_PATH=-L/my/favorite/path/lib

    Note you can add multiple paths if, for example, libxml and libsbml are in different locations:

    LINK_SEARCH_PATH=-L/my/favorite/path/lib -L/another/path/lib

- From the SBMLconverter directory, type: make

- You should now have an executable named sbml2stochkit in the SBMLconverter/bin directory

Converting an SBML model to StochKit2 format

The converter creates an executable called "sbml2stochkit" that takes at most two arguments: the input path to the sbml file and the output path to the StochKit2 model file that the converter will create. For example, if I have an sbml file named "mySBMLmodel.xml" and I want to convert it to StochKit model format with the name "myStochKitModel.xml" in the tools/SBMLconverter directory, then from the tools/SBMLconverter directory I can call:

bin/sbml2stochkit mySBMLmodel.xml myStochKitModel.xml

If the output file name is not given, the default name is "<input file name without .xml>.stochkit.xml". So if you call:

bin/sbml2stochkit mySBMLmodel.xml

it creates an output file named "mySBMLmodel.stochkit.xml" in the same directory as the file "mySBMLmodel.xml".

If no argument is given, i.e. you call

bin/sbml2stochkit

the executable will return a message that says

Please input the SBML file name:

You can input the filename right now. After you hit enter, the executable will ask you if you want to input the output file name,

Do you want to input the output file name (y or n):

If you type "y" or "yes", you can input the output file after the message,

Type in the file name:

If you choose "n" or "no", the executable will generate the output file with the default name.

The converter executes the sbml format verification when it reads the data file, so you may receive error or warning messages if the data file does not follow the sbml format perfectly. However, most errors and warnings are not critical,and the converter generates an output file even though error or warning messages appear. The verification messages are written in a log file, which is in the same directry as the generated .xml file and the name of the log file is " <outputfilename>.log". When the SBML format data file does not have all the information required by StochKit2, the converter also provides warnings to help you locate the missing parts. After running sbml2stochkit, always check the created file to ensure it is correct.

Currently StochKit does not support the following features of SBML.

Multiple compartments
Function definition
SBML format event
Constraint
Initial assignment

Rule
Boundary condition for a species
Unit definition
Parameters with the same name
Modifier

Explanations of the warnings

- **No model name is provided.**
  In the data file, the component <model /> does not have the attribute "name".
- **Number of reactions is zero.**
  The data file includes no reaction in <listOfReactions /> tag or the tag has no element.
- **Number of species is zero.**
  The data file includes no species in <listOfSpecies /> tag or the tag has no element.
- **Warning: The model has no compartment. You can ignore this warning if all the reactions are assumed to be in one compartment and the initial population are given in the form of initial amount**
  The data file has no <listOfCompartments/> tag or the tag has no element. But it does not matter if all the reactions are assumed to be in one compartment and the initial population are given in the form of initial amount
- **The size of the compartment 'COMPARTMENT NAME' is unknown. If the species' initial population are give in the form of initial amount (not initial concentration), just ignore this warning**
  In the data file, the compartment 'COMPARTMENT NAME' in the compartment list <listOfParameters/> does not have the attribute "size" (or "volume" for Level 1), which is necessary when the population is given in the form of concentrition.
- **The units of the size of compartment 'COMPARTMENT NAME' is not set.**
  In the data file, the compartment 'COMPARTMENT NAME' in the compartment list <listOfParameters/> does not have the attribute "units", which may be necessary when the population is given in the form of concentration.
- **The i th global parameter missed its id.**
  In the data file, the i th parameter in the global parameter list <listOfParameters/> does not have the attribute "id" (or "name" for SBML Level 1).
- **The value of the i th global parameter 'PARAMETER NAME' is not set.**
  In the data file, the i th parameter 'PARAMETER NAME' in the global parameter list <listOfParameters/> does not have the attribute "value".
- **Reaction i missed its id.**
  In the data file, the i th reation in the reaction list <listOfReactions/> dosen't have the attribute "id" (or "name" for Level 1).
- **The i th reaction 'REACTION NAME' does not have kineticLaw.**
  In the data file, the i th reaction 'REACTION NAME' in the reaction list <listOfReactions/> does not have the component "kineticLaw".
- **The j th reactant in the i th reaction 'REACTION NAME' missed its id.**
  In the data file, the j th reactant in the reactant list <listOfReactants/> of the i th reaction 'REACTION NAME' in the reaction list <listOfReactions/> does not have the attribute "species".
- **The j th product in the i th reaction 'REACTION NAME' missed its id.**

In the data file, the j th product in the product list <listOfProducts/> of the i th reaction 'REACTION NAME' in the reaction list <listOfReactions/> does not have the attribute "species".

- **The j th parameter in the i th reaction 'REACTION NAME' missed its id.**
  In the data file, the j th parameter in the local parameter list <listOfParameters/> of i th reaction 'REACTION NAME' in the reaction list <listOfReactions/> dosen't have the attribute "id" (or 'name' for Level 1).
- **The value of the j th parameter 'PARAMETER NAME' in the i th reaction 'REACTION NAME' is not set**.
  In the data file, the j th parameter in the local parameter list <listOfParameters/> of i th reaction 'REACTION NAME' in the reaction list <listOfReactions/> dosen't have the attribute "value".
- **The i th species in the species list missed its id.**
  In the data file, the i th species in the species list <listOfSpecies/> does not have the attribute "id" (or 'name' for Level 1).
- **Initial amount of the i th species 'SPECIES NAME' is negative.**
  In the data file, the attribute "initialAmount" of the i th species in the species list <listOfSpecies/> has a negative value.
- **The initial polulation of the i th species 'SPECIES NAME' is given in the form of initial concentration**.
  In the data file, the attribute "initialConcentration" of the i th species in the species list <listOfSpecies/> is given rather than the attribute "initialAmount".
- **Initial concentration of the i th species 'SPECIES NAME' is negative.**
  In the data file, the attribute "initialConcentration" of the i th species in the species list <listOfSpecies/> has a negative value.
- **The units of the initial concentration of the i th species 'SPECIES NAME' is not set.**
  In the data file, the i th species in the species list <listOfSpecies/> does not have the attribute "units", which may be necessary when the population is given in the form of concentrition.
- **Initial amount and initial concentration of the i th species 'SPECIES NAME' are unknown.**
  In the data file, the i th species in the species list <listOfSpecies/> does not have the attributes "initialAmount" and "initialConcentration".