Documentation for SBML to dot converter.

Summary:
This converter can be used to convert a SBML model into dot, a graph support format. Additionally, an option is available for generating a graphical representation in the following formats: svg, png and jpg. Mathematical layout and image generation is done by GraphViz. The conversion is mainly based on the listOfSpecies and listOfReaction. Besides, SBGN and MIRIAM annotations accuracy enhance glyph diversity and relevancy. Please note that SBGN annotations are the most useful in the conversion.

public void **dotExport**(SBMLDocument sbmlDocument, PrintWriter out)
This is the main function for the export in dot format. We use jSBML to load the SBML model and then extract the lists of Species and Reactions which are the only relevant things for the conversion. The main function is built in two parts, one for the dot file generation, the other one for the image generation if a second valid argument is given.

The list of Reactions is analyzed for cloning. We will count the number of arcs to and from each Species and store these informations in a Map. This is the purpose of:
private void **addCardinality**(ListOf<? extends SimpleSpeciesReference> listOf)

The beginning of the graph object is then printed. The number of Species and Reactions are checked: if there is no Species or Reactions or if there too much Species or Reactions the conversion is aborted.

Once these few check steps are completed, we then loop over first the Species. For each of them a dot node will be written if their cardinality does not exceed the number of edges allowed on a single node. No node will be drawn for the empty set at this stage.

For each Species a shape will be retrieved using the function *getShape*() of the *SBGNUtils* class. To use this function, a *SBGNUtils* object converter has been called with dot as parameter, therefore calling this method will return dot shapes. These shapes are based on the SBO terms and annotations found in the SBML model. Once we retrieve a SBGN class with the SBO term or the annotations, a mapping is done to dot.

The next step is to loop over the list of Reactions in order to write process nodes and their associated arcs. First, once a dot shape is retrieved (with the same procedure as a Species) for a Reaction, the process node is printed in dot format.

Finally, arcs will be drawn. There 2 types of arcs: arcs can come from a Species to a process nodes (incoming arcs) or from a process node to a Species (outgoing arcs). Incoming arcs classes can be retrieved by looping over the list of reactants and modifiers whereas the list of products has to be looped over for outgoing arcs.

Thus, empty sets do appear here and arcs from and to them are printed in the dot file if there is no reactant (source) or no product (sink).

Firstly reactants are looped over and their arcs are drawn. If one of the reactants appear to be a empty set, then a empty set node is created. Arcs can have a normal arrow tail if the reaction is reversible or be without if not. There is no cardinality label created for consumption arcs. Secondly products are looped over and empty sets and simple edges are printed. Finally for each modifiers an arc is drawn.

Cloning

No nodes duplication are currently implemented in the SBML to dot converter. Cloning rules are not clearly established and no methods has been implemented yet. However, it has been suggested that cloning can occur when a Species node possess five or more edges and if its class is eligible for cloning regarding SBGN specifications.