
sbml2hyb Documentation

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The sbml2hyb tool is an stand-alone executable application for SBML compatible hybrid modelling. The tool is written in Python and is intended as an interface to convert existing [SBML](#) models into a hybrid model (combines mechanistic equations and ML techniques). Below see the proposed pipeline in Figure 1. The new internal hybrid model format HMOD (intermediate format — enables communication between the essential components of the mechanistic and hybrid models) can be translated to SBML and vice-versa. See [HMOD](#) format example.

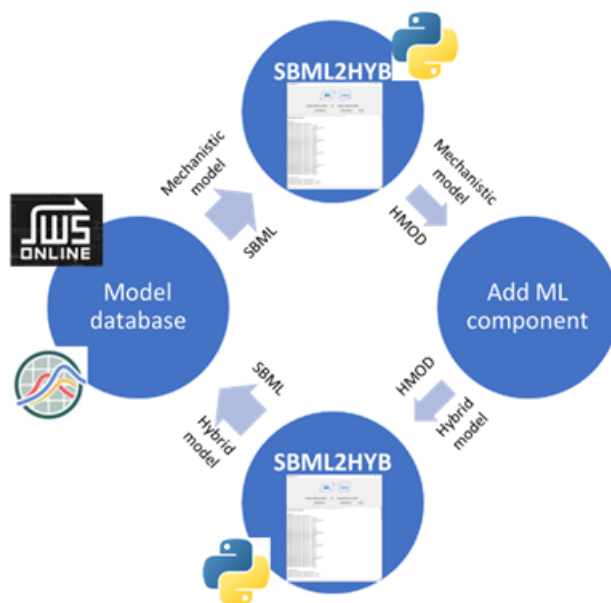


Fig. 1: **Figure 1. Overview of the sbml2hyb pipeline.**

Source code available [HERE](#).

USING SBML2HYB

Here is an example of a SBML hybrid model ([Chassagnole case study](#)) built with **sbml2hyb**:

After launching `sbml2hyb` (see installation instructions), the following graphical user interface (GUI) will be open (Figure 2). Once the simple GUI window opens, click the “*Translate SBML file*” button (see Figure 2), and browse to specify the SBML model file (here the mechanistic model example is taken from Biomodels database, [BIOMD0000000066](#)) you want to convert. Add then the information of the neural network component into the model (click “*Add ML*” button). Once you do this, select the “*Inputs*” (select all) and “*Outputs*” (`vm5`, `vm4f`, `vm3f`, `vm2f`, `vm11`, `knadph` and `katpase`) options, and the [Keras](#) neural network file for this case study (Figure 3) to be added to the mechanistic model. After this, click the “*Confirm*” buttons. Finally, the hybrid model generated in HMOD format is reconverted in SBML by clicking the “*Translate HMOD file*” button and then “*Confirm*” button (Figure 4). To save the final hybrid SBML model file, click “*Save file*” button (Figure 5).

NOTE: To generate the Keras H5 file that serves as a blueprint of the machine learning segment of the hybrid model, follow these instructions:

- 1- To generate an H5 file that serves as a blueprint of the machine learning segment of a hybrid model, the Keras library from Tensorflow, Python is used. After importing this library, the first step is to initialize a sequential artificial neural network (ANN) model via the “*Sequential*” function in the form “`model=Sequential()`”, where `model` is a variable containing the model information.
- 2- This is followed with adding any number of hidden layers with a hyperbolic tangent activation function via the “*add*” function. This function should be written for each layer in the form: “`model.add(Dense(NH, activation='tanh', input_shape(Nprev)))`”, where `NH` is the number of hidden nodes the user desires in this layer and `Nprev` is the number of nodes on the previous layer. For the first layer, `Nprev` must correspond to the number of desired network inputs.
- 3- After the user is satisfied with the number of hidden layers, the final layer should be written in the form: “`model.add(Dense(Nout))`”, where `Nout` is the number of outputs the user wishes the machine learning section to have.
- 4- With the model finalized, it can be saved to an H5 file using the “*save*” function in the form: “`model.save('filename.h5')`”

See also this example as [notebook](#).

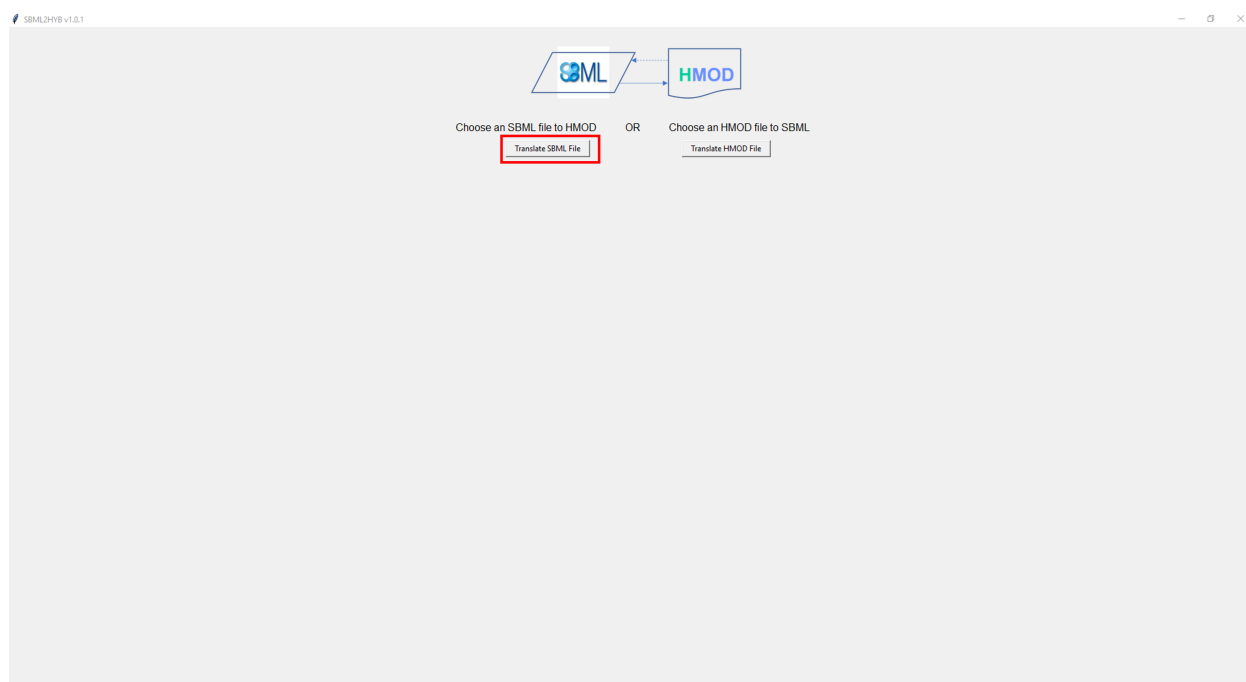


Fig. 1: Figure 2. The main GUI of sbml2hyb.

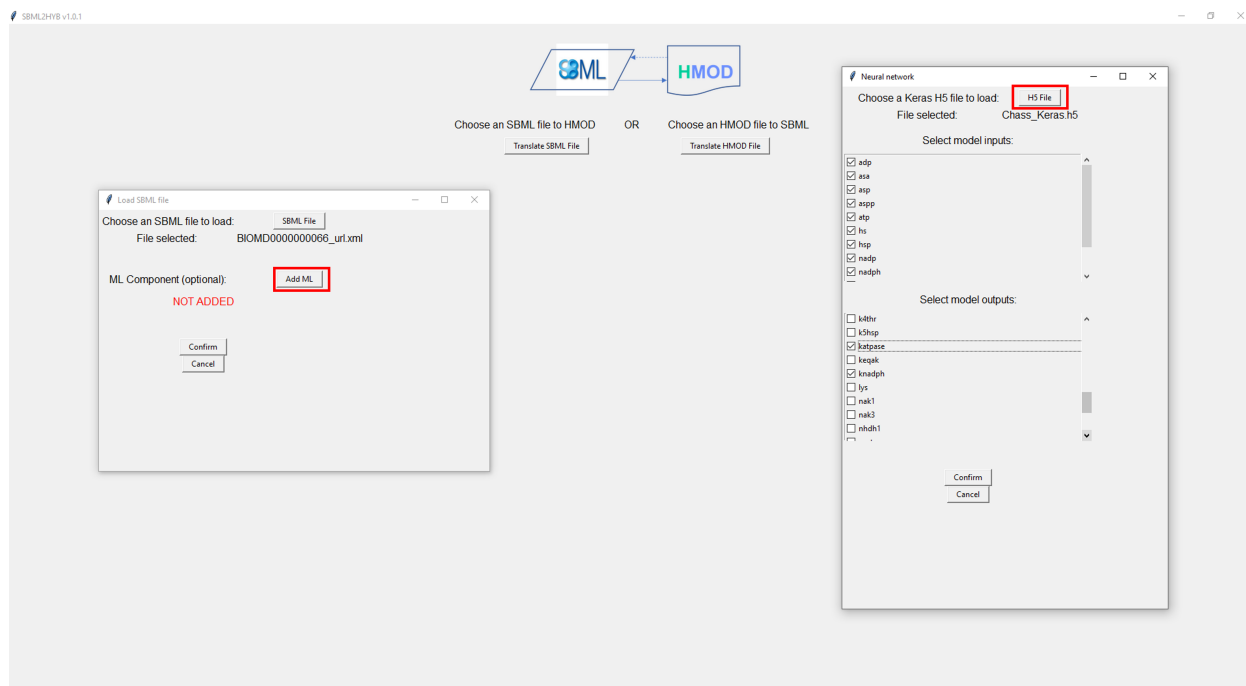


Fig. 2: Figure 3. Screenshot of the ML component panel. Here, the user can select the input/output variables and the Keras neural network file in H5 format, which is automatically added to the mechanistic model.

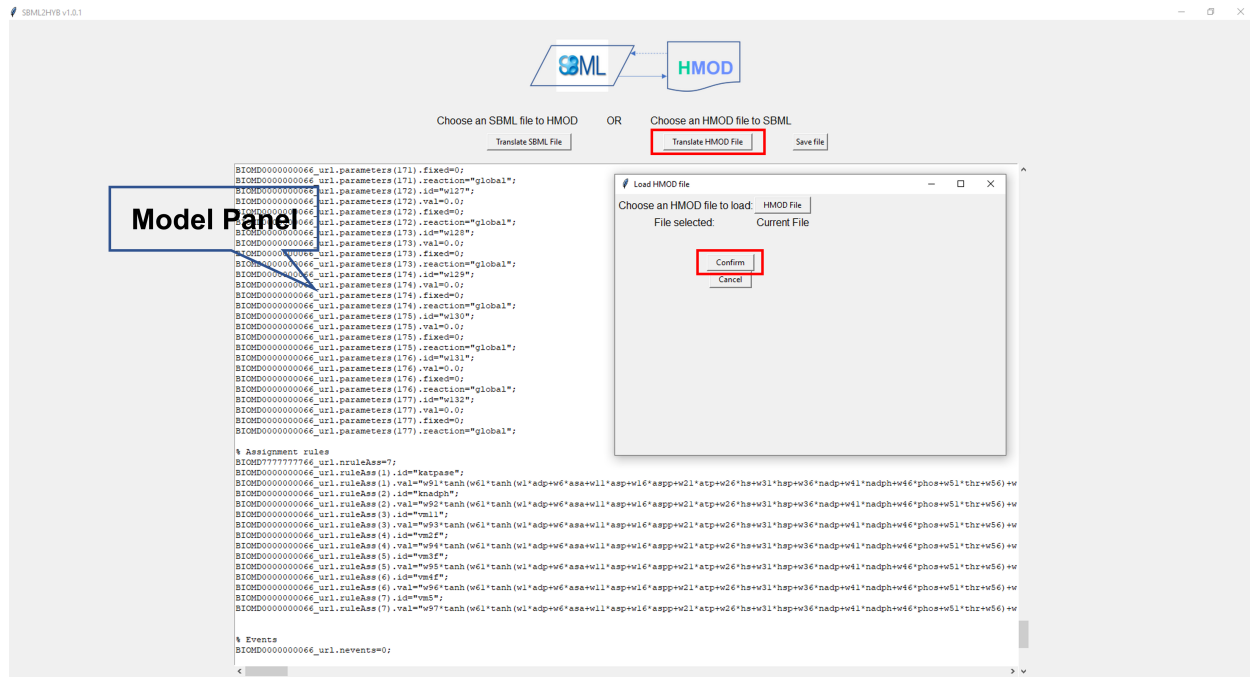


Fig. 3: Figure 4. Print screen of the hybrid model in HMOD format that can be converted to SBML.

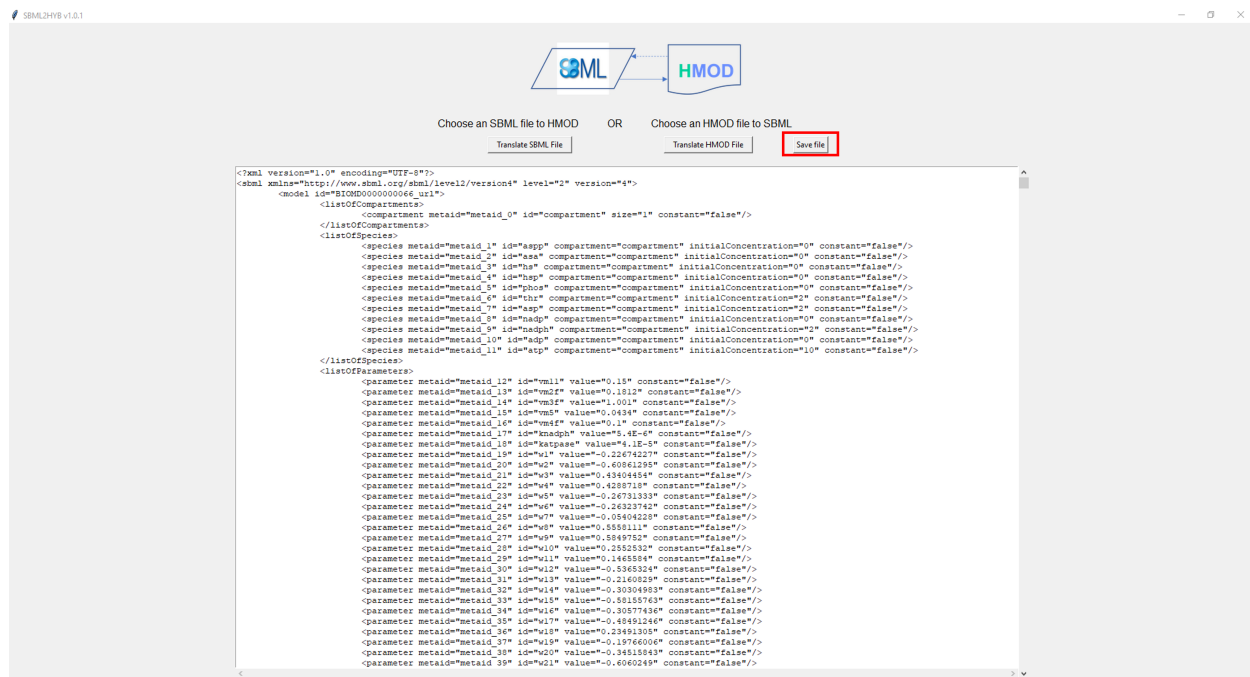


Fig. 4: Figure 5. Print screen of the final hybrid model in SBML.

INSTALLATION

The sbml2hyb package is available from pypi and can be installed via:

```
$ pip install sbml2hyb
```

For detailed installation instructions please see <https://github.com/r-costa/sbml2hyb>.

HOW TO CITE SBML2HYB

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LICENSE

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