1 First example: The Schlogl model

1.1 Deterministic model

The Schlo?gl model is a quite famous example of a simple reaction network which exhibits bi-stability, i.e. the solution strongly depends on the initial conditions and parameters, converging to one of the two stable states. The system of Ordinary Differential Equations (ODEs) is the following (probably online might exist other formulation):

$$\begin{aligned}\frac{dB1}{dt} &= -c1/2 * B1 * X1^2 + c2/6 * X1^3 \\ \frac{dX1}{dt} &= +c1/2 * B1 * X1^2 - c2/6 * X1^3 + c3 * B2 - c4 * X1 \\ \frac{dB2}{dt} &= -c3 * B2 + c4 * X1\end{aligned} \tag{1}$$

where:

$$\begin{aligned} c1 &= 3 \cdot 10^{-7}, \\ c2 &= 10^{-4}, \\ c3 &= 10^{-3}, \\ c4 &= 3.5 \qquad . \end{aligned}$$

Therefore we can represent these equations through the following Petri Net (PN) model:

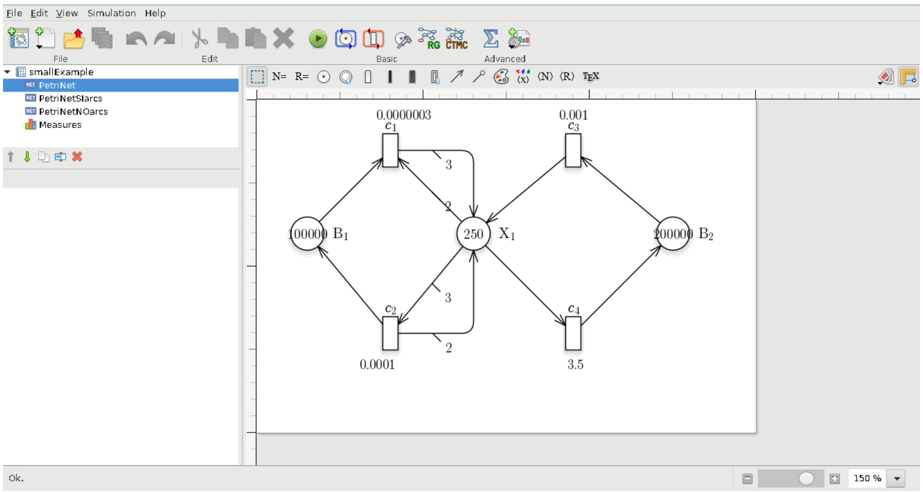

Figure 1: The PN model corresponding to the Schlogl model.

Since the molecular numbers for the species B1 and B2 are kept at constant values, B1 $= 10^5$ and B2 $= 2 \times 10^5$, then we can reduce the system of ODEs 1 in just one equation with the following Petri Net (PN) graph:

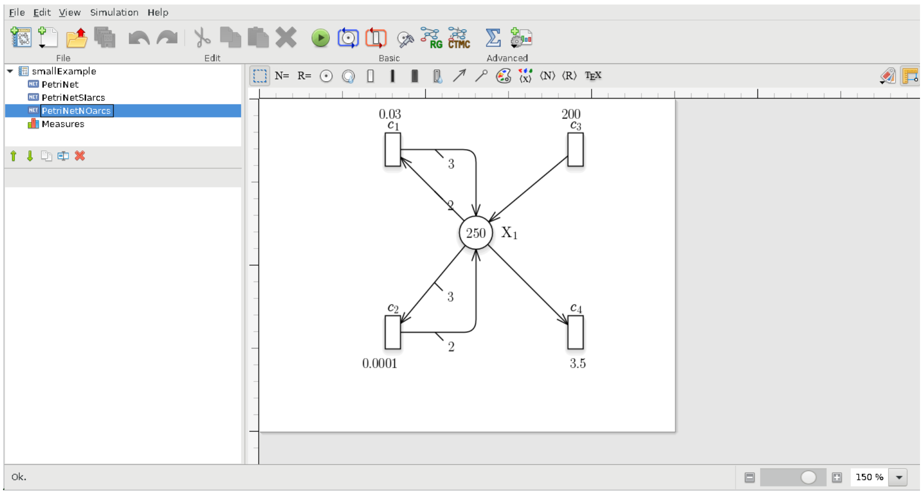

Figure 2: The PN model corresponding to the reduced Schlogl model.

To obtain the two stable states in the deterministic state, we took the initial condition $X(0) = 248$ for the lower stable state and $X(0) = 247$ for the upper stable state.

How to generate the file storing te ODEs system.

1. First of all the PN graph has to be drawn.
2. Export then net as GreatSPN format, let us suppose to call the file: "PNexample".
3. From terminal you can:
   - *PN2ODE.sh "PNexample" -M*
     if it is interested to the C++ solver, where the option "-M" is settled to have the reactions syntax as Mass Action law.
     In this case, the simulation and the solution of the ODEs system, that will be saved in a file called "solution"(second input), corresponding to PNexample is obtained through:
     ./PNexample.solver solution -ftime FinalTime -stime TimeStepSize

     P.S. To see all the options available as inputs to the solver:
     ./PNexample.solver
   - *PN2ODE.sh "PNexample" -M -R*
     if it is interested to the R file. Here you have just to fix the hini, FinalTime and TimeStepSize value before running the R script.

1.2 Stochastic model

For the stochastic model, te PN model is the same, it is not necessary to modify the graph but just the name of the solver to exploit:

./PNexample.solver solution -ftime FinalTime -stime TimeStepSize -type SSA -runs 500

In this case starting with X(0)=248 it is possible to observe that the trajectories spontaneously switch between the two stable states.