Using the SACNA package - reverse APED model

The purpose of this document is to give a short tutorial for the SACNA package.
Let’s start by bringing the package functions to this notebook.

```
In[]:= Quiet[ClearAll["Global`*"]];
       Quiet[Remove["Global`*"]];
       SetDirectory[NotebookDirectory[]];

       Quiet[Get["../SACNA.wl"]]
```

Now let’s input the reactions and rates lists of this model. If we input the rates list as an empty list, SACNA will assign rates by default in the order of the list (the first reaction has constant k1 and so on). Reactions must be in terms of D-species, L-species, Z-species (achiral species), and the empty specie N1.

```
In[]:= reactions = {"L1->L2", "L2->L1", "L2+L1->L3", "L3->L2+L1", "D2+L1->D4", "D4->D2+L1",
          "L3->2L1", "2L1->L3", "L4->L1+D1", "L1+D1->L4", "L4->D3", "D3->L4"};
       rates =
         {};
```

Note that we are not writing all the reactions, only it is left the dual reactions. If we use the function `ClausuraDual`, we can get all the reactions. This is done by default in the `RunSemiAlgebraicAnalysis` function.

```
In[]:= Quiet[ClausuraDual[reactions]]

Out[]= {L1->L2, L2->L1, L1+L2->L3, L3->L1+L2, D2+L1->D4, D4->D2+L1, L3->2L1, 2L1->L3,
        L4->D1+L1, D1+L1->L4, L4->D3, D3->L4, D1->D2, D2->D1, D1+D2->D3, D3->D1+D2,
        D1+L2->L4, L4->D1+L2, D3->2D1, 2D1->D3, D4->D1+L1, D1+L1->D4, D4->L3, L3->D4}
```

Now we can run the semialgebraic analysis of the model by using the `RunSemiAlgebraicAnalysis` function. The first parameter corresponds to the reactions’ list, the second parameter corresponds to the rates’ list, and the last parameter corresponds to time in seconds (the Collins’ algorithm may take so much time to find a solution). The function will ask for the Routh-Hurwitz condition number. Considering the first and last numbers will be faster, because this conditions are shorter than the others. This example give us 4 Routh-Hurwitz conditions. Let’s begin with the first condition.

In[ ]:=
```
time = 60;
cadSolutions = RunSemiAlgebraicAnalysis[reactions, rates, time]
```

Out[ ]=
```
False
```

The first condition cannot be satisfied. As mentioned before, let’s try with the last condition (in this case, the fourth one).

```
time = 600;
cadSolutions = RunSemiAlgebraicAnalysis[reactions, rates, time]
```

```
Intento de buscar un ejemplo sin CAD

Se alcanzó el tiempo impuesto sin llegar a una solución
```

Out[ ]=
```
Se alcanzó el tiempo impuesto sin llegar a una solución
```

In this case, the algorithm may take so much time finding the solution (if it exists). For these cases, SACNA provides the function RunSemiAlgebraicAnalysisWithInitialValues. We can input values for some parameters, in order to speed up the computations.

In[∘]:=
```
time = 60;
initialValues = {D1 → 1, D2 → 1, k1 → 1, k2 → 1,
   k3 → 1, k4 → 30761/1401, k9 → 1, k10 → 1, k11 → 1, k12 → 3/2};
cadSolutions = RunSemiAlgebraicAnalysisWithInitialValues[
  reactions, rates, time, initialValues]
```

Out[∘]=

$$\Bigg(0 < D3 < \frac{137054226}{4319775625} \&\& D4 == \frac{65725\,D3}{5604} \&\&$$
$$\Bigg(\Bigg(\frac{-8406\,D3 - 12609\,D3^2 + 8406\,D3\,D4}{8406\,D3 - 5604\,D4 + 139856\,D3\,D4 - 5604\,D4^2} < k5 < \frac{-8406\,D3 - 12609\,D3^2 + 8406\,D3\,D4}{8406\,D3 - 2802\,D4 + 65725\,D3\,D4} \&\&$$
$$k6 == \frac{2 + 3\,D3 - 4\,D4 + 2\,k5}{2\,D4} \&\& \frac{2802 - 65725\,D3 + 2802\,D4}{2802\,D3} < k7 <$$
$$(11776806 - 552484350\,D3 + 23553612\,D4 + 172384644\,k5 - 4319775625\,D3\,k5 + 184161450\,D4\,k5 + 11776806\,k6 - 552484350\,D3\,k6 + 23553612\,D4\,k6) \Big/ (23553612\,D3 - 7851204\,k5 + 184161450\,D3\,k5 + 23553612\,D3\,k6) \&\&$$
$$k8 == \frac{-2802 + 65725\,D3 - 2802\,D4 + 2802\,D3\,k7}{2802}\Bigg) \;||$$
$$\Bigg(k5 \geq \frac{-8406\,D3 - 12609\,D3^2 + 8406\,D3\,D4}{8406\,D3 - 2802\,D4 + 65725\,D3\,D4} \&\& k6 == \frac{2 + 3\,D3 - 4\,D4 + 2\,k5}{2\,D4} \&\&$$
$$k7 > \frac{2802 - 65725\,D3 + 2802\,D4}{2802\,D3} \&\& k8 == \frac{-2802 + 65725\,D3 - 2802\,D4 + 2802\,D3\,k7}{2802}\Bigg)\Bigg)\Bigg) \;||$$
$$\Bigg(\frac{137054226}{4319775625} \leq D3 < \frac{321215676}{4872259975} \&\& D4 == \frac{65725\,D3}{5604} \&\&$$
$$k5 > \frac{-8406\,D3 - 12609\,D3^2 + 8406\,D3\,D4}{8406\,D3 - 5604\,D4 + 139856\,D3\,D4 - 5604\,D4^2} \&\&$$
$$k6 == \frac{2 + 3\,D3 - 4\,D4 + 2\,k5}{2\,D4} \&\&$$
$$\frac{2802 - 65725\,D3 + 2802\,D4}{2802\,D3} < k7 <$$
$$(11776806 - 552484350\,D3 + 23553612\,D4 + 172384644\,k5 - 4319775625\,D3\,k5 + 184161450\,D4\,k5 + 11776806\,k6 - 552484350\,D3\,k6 + 23553612\,D4\,k6) \Big/ (23553612\,D3 - 7851204\,k5 + 184161450\,D3\,k5 + 23553612\,D3\,k6) \&\&$$
$$k8 == \frac{-2802 + 65725\,D3 - 2802\,D4 + 2802\,D3\,k7}{2802}\Bigg)$$

The algorithm found a solution. This is a particular solution of the system, but it is better than nothing. There is not an specific way of choosing the parameters and their initial values, that’s why this sould be done as a last resource.

Let’s find some particular solutions by using the `FindInstance` command. Note that the solution doesn’t contain an expression for the L-species. It’s because we are assuming the racemic condition.

In[ ]:=
```
numberOfSamples = 10; (*feel free to change*)
samplesList = FindInstance[cadSolutions,
                          encuentra caso
    DeleteCases[DeleteDuplicates@Cases[cadSolutions, _Symbol, Infinity],
    elimina casos  elimina repeticiones   casos                        infinito
     Alternatives @@ {GreaterEqual, Greater, Less, LessEqual}], numberOfSamples];
     alternativas     mayor o igual    mayor    menor menor o igual
sampleNumber = 8;  (*feel free to change*)
samplesList[[sampleNumber]]
```

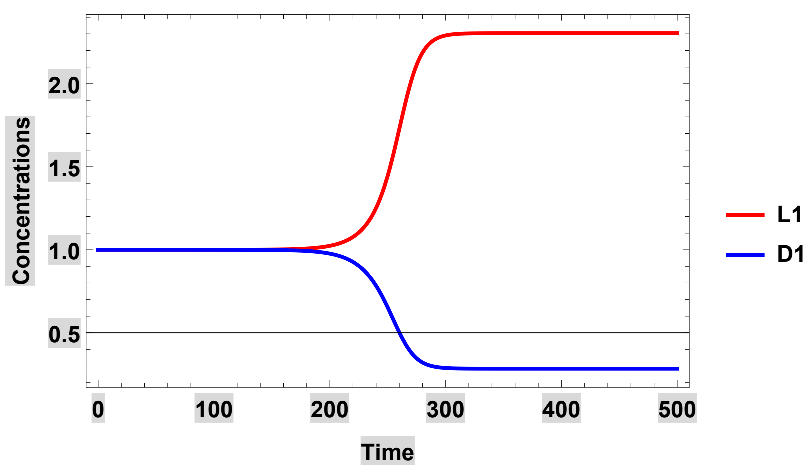
Out[ ]=

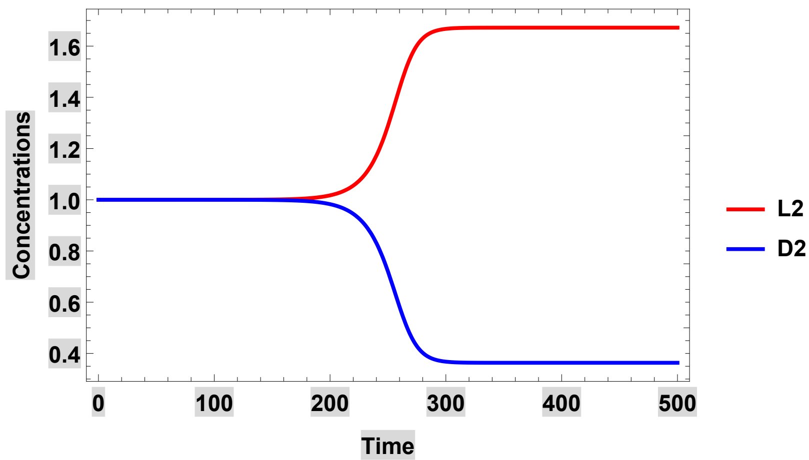
$$\left\{D3 \to \frac{1343}{29\,269},\ D4 \to \frac{88\,268\,675}{164\,023\,476},\ k5 \to 101,\ k6 \to \frac{194\,884\,076}{1\,038\,455},\ k7 \to \frac{41}{3},\ k8 \to \frac{27\,102\,883}{164\,023\,476}\right\}$$

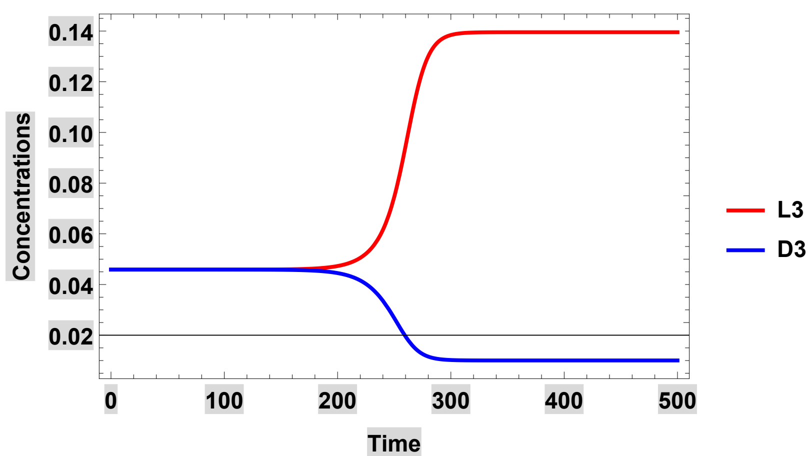
Now we are ready to using the SACNA’s system simulator with the `ReactionSystemSimulator` function. The simulation time depends on the sample. The user has to set it up.

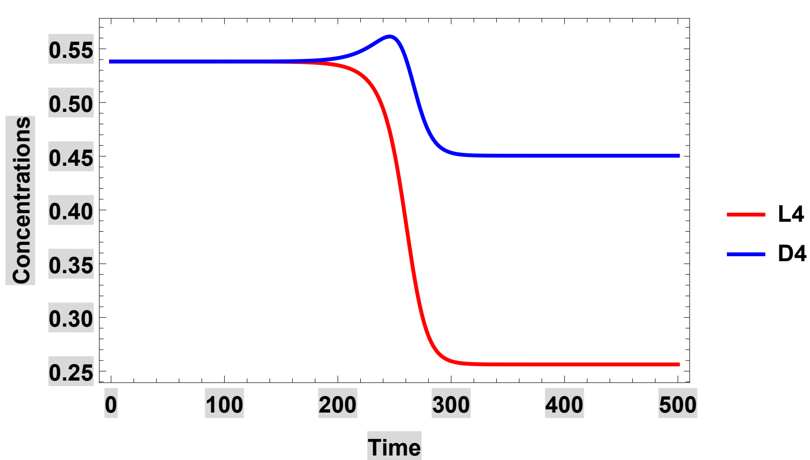
In[ ]:=
```
simulationTimeMin = 0;
simulationTimeMax = 500; (*feel free to change*)
graficss = ReactionSystemSimulator[reactions,
    rates, Join[samplesList[[sampleNumber]], initialValues],
           junta
    0.000001, t, simulationTimeMin, simulationTimeMax];
```

```
Species Concentrations Graphic
```









SACNA also allows to export a simulation results to ChemKinLator simulator files with the function `ExportToChemKinLator`.

In[∘]:=

```
content = ExportToChemKinLator[reactions, rates, samplesList[[sampleNumber]],
    1/1000000000000000, 1/1000000000000000, 0, simulationTimeMax, 1000];
```

... Export: First argument $Canceled is not a valid file specification.

We could try to do the same with the second and third Routh-Hurwitz condition, but in this case it could take a lot of time.

The user would like to know which rate constant corresponds to some reactions. It can be done with the function `GetReactionsAndRates`.

In[ ]:=
```
GetReactionsAndRates[reactions, rates] // MatrixForm
```
forma de matriz

Out[ ]//MatrixForm=

L1->L2	k1
L2->L1	k2
L1+L2->L3	k3
L3->L1+L2	k4
D2+L1->D4	k5
D4->D2+L1	k6
L3->2L1	k7
2L1->L3	k8
L4->D1+L1	k9
D1+L1->L4	k10
L4->D3	k11
D3->L4	k12
D1->D2	k1
D2->D1	k2
D1+D2->D3	k3
D3->D1+D2	k4
D1+L2->L4	k5
L4->D1+L2	k6
D3->2D1	k7
2D1->D3	k8
D4->D1+L1	k9
D1+L1->D4	k10
D4->L3	k11
L3->D4	k12