On the Package ReactionKinetics.wl

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Preliminaries

In[1]:=
```
SetDirectory[NotebookDirectory[]];
```

In[2]:=
```
SetOptions[#, AxesStyle → Arrowheads[Automatic]] & /@
  {ContourPlot, DateListPlot, Plot, ListLinePlot, ListPlot, ListLogPlot,
   LogLinearPlot, LogPlot, ParametricPlot, Plot3D, RegionPlot};
SetOptions[GraphPlot, DirectedEdges -> True, VertexLabeling → All];
```

In[4]:=
```
LaunchKernels[];
```

In[5]:=
```
Needs["ReactionKinetics`"]
```

```
ReactionKinetics Version 1.0 [March 25, 2018] using
  Mathematica Version 11.3.0 for Microsoft Windows (64-bit) (March 7,
  2018) (Version 11.3, Release 0) loaded 12 April 2018 at 11:05 TimeZone
GNU General Public License (GPLv3) Terms Apply.

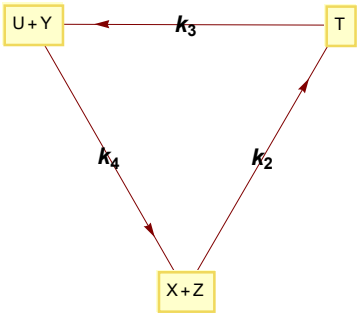
Please report any issues, comments, complaint related to ReactionKinetics at
jtoth@math.bme.hu, nagyal@math.bme.hu or dpapp@iems.northwestern.edu
```

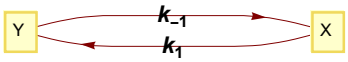
In[6]:=
```
ClearAll[format, figurexp];
format[x_, options___] :=
 Thread[x → (Style[#, SingleLetterItalics → False, options] & /@ x)];
figurexp[filename_, picturename_] := Export[
  "d:\\__Springer\\SpringerAktualis\\Figures\\" <> filename <> ".png", picturename]
```

What is formal reaction kinetics?

Feinberg-Horn III

```
ShowFHJGraph[FHIII = {"X" ⇔ "Y", "X" + "Z" → "T" → "Y" + "U" -> "X" + "Z"},
  {k1, k-1, k2, k3, k4}, EdgeLabeled → True, ImageSize → 200] /. {kw_ -> Style[kw, Bold, 12]}
```





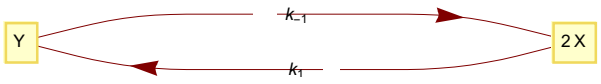

```
RightHandSide[{FHIII}, {k1, k-1, k2, k3, k4}, {x, y, z, t, u}] // Column
```

$$y\,k_{-1} - x\,k_1 - x\,z\,k_2 + u\,y\,k_4$$
$$-y\,k_{-1} + x\,k_1 + t\,k_3 - u\,y\,k_4$$
$$-x\,z\,k_2 + u\,y\,k_4$$
$$x\,z\,k_2 - t\,k_3$$
$$t\,k_3 - u\,y\,k_4$$

How to say anything about stationary points and dynamic behavior? Let us take a simpler example.

Dimerization

```
ShowFHJGraph[dimer = {2 "X" ⇔ "Y"}, {k1, k-1}, EdgeLabeled → True]
```

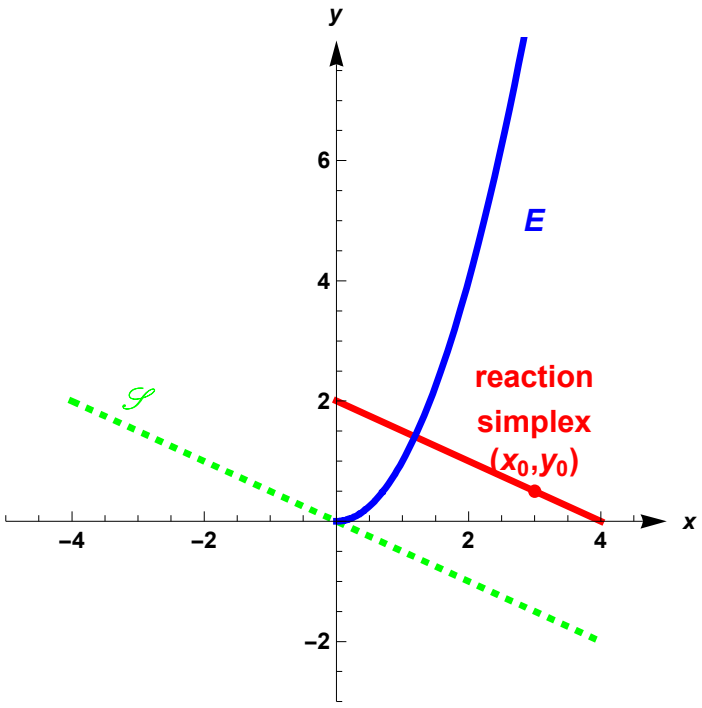



```
Column@First@DeterministicModel[dimer, {k1, k-1}, {x, y}]
```

$$x'[t] == -2\,k_1\,x[t]^2 + 2\,k_{-1}\,y[t]$$
$$y'[t] == k_1\,x[t]^2 - k_{-1}\,y[t]$$

In[ ]:=
```
statpoints = ParametricPlot[Evaluate[
    Flatten[{x, y} /. Rest[StationaryPoints[{2 "X" ⇔ "Y"}, {1, 1}, {u, v}, {x, y}]]] /.
     (Last[First[GammaLeftNullSpace[{2 "X" ⇔ "Y"}, {u, v}, {x, y}]]] /. Plus → Rule)],
  {v, 0, 10}, PlotStyle → Directive[{Blue, Thickness[0.01]}],
  Prolog → {Directive[{Green, Dashed, Thickness[0.01]}],
    Line[{{-4, 2}, {4, -2}}], Directive[{Red, Dashing[{}], Thickness[0.01]}]
    , Line[{{0, 2}, {4, 0}}], PointSize[0.02], Point[{3, 1 / 2}], Green,
    Text[Style["S", FontFamily → "Kunstler Script", Bold, 16], {-3, 2}],
    Red, Text[Style["reaction\nsimplex", Bold, 16], {3, 2}],
    Text[Style["(x0,y0)", Bold, 16], {3, 1}], Blue,
    Text[Style["E", Italic, Bold, 16], {3, 5}]},
  AspectRatio → 1, PlotRange → {{-5, 5}, {-3, 8}},
  AxesLabel → (Style[#, Bold, Italic, 12] & /@ {"x", "y"}),
  TicksStyle → Directive[Black, Bold, 12]]
```

Out[ ]=



Why does it behave so well?

```
ReactionsData[{2 "X" ⇔ "Y"}]["deficiency"]
```

δ=N-L-S=2-1-1=0

```
WeaklyReversibleQ[{2 "X" ⇔ "Y"}]
```

True

Suppose that the deficiency ($N - L - S$) of a reaction is zero. Then:

1. No nontrivial periodic solutions of the induced kinetic differential equation can exist.

2. Furthermore,

a. If the reaction is not weakly reversible then it cannot have a positive stationary point, no matter what form the kinetic has.

b. If the reaction is weakly reversible and the kinetic is of the mass action form then with any choice of positive rate constants (i.e. with any mechanism built on the given reaction):

i. There exists in each positive stoichiometric compatibility class exactly one positive stationary concentration.
ii. Each of the positive stationary concentrations is **relatively** asymptotically stable relative to the stoichiometric compatibility class in which it resides.

Returning to FH III

In[•]:=
```
FHIII = {"X" ⇔ "Y", "X" + "Z" → "T" → "U" + "Y" → "X" + "Z"};
```

```
WeaklyReversibleQ[{FHIII}]
```

```
True
```

```
ReactionsData[{FHIII}]["deficiency"]
```

δ=N−L−S=5−2−3=0

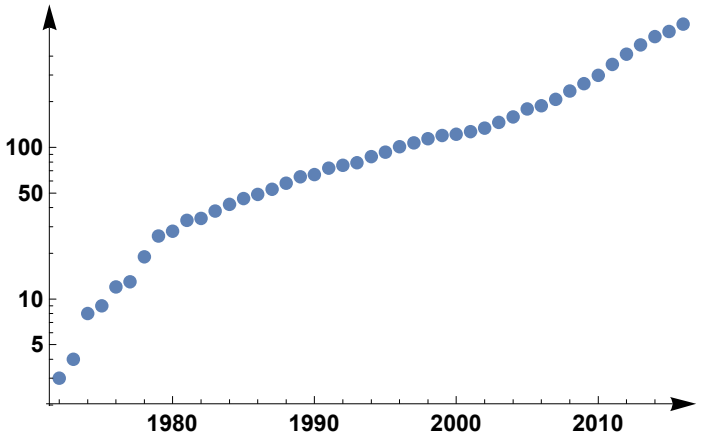
Citations to the paper by Horn and Jackson

Data collected manually from scholar.

```
cit = {3, 4, 8, 9, 12, 13, 19, 26, 28, 33, 34, 38, 42, 46, 49,
    53, 58, 64, 66, 73, 76, 79, 87, 93, 101, 107, 114, 120, 122, 127, 134,
    146, 159, 179, 188, 207, 235, 263, 298, 353, 412, 475, 537, 581, 649};
```

The logarithm of the number of citations of Horn and Jackson (1972) up to a certain year. Note the three phases: Up to 1980, and after 2002 and in between.

```
ListLogPlot[Transpose[{Range[1972, 2016], cit}],
 PlotStyle → Directive[PointSize[Large]], TicksStyle → Directive[Black, Bold, 12]]
```



Our early history

Stochastic simulation since 1972 (Érdi, P.; Hárs, V., Sipos, T.; Tóth, J.)

Mathematica codes for reaction kinetics since 2002 (Nagy A. L.; Nagy, I.; Papp, D.; Rospars, J.-P.; Tóth, J.

and students :) such as Bányász, K.; Berencsi K.; Eszes, D.; Halmschlager A.; Kovács, B.; Ladics, T.; Sipos Szabó E.; Szabó A., Takács B.; Varga N.; Várdainé Kollár J.; Zsámboki B.; Vizi Zsolt (Szeged))

Numerics and beyond (or before): What can be done with the computer?

Goals

Calculations of conditions of known theorems and of our results to help the chemist in case if they are not feasible manually.

Solving induced kinetic differential equations, simulating the stochastic model, estimating parameters.

Physical circumstances

```
In[ ]:= lvgenuine = ReactionsData[{"Lotka-Volterra"}];
In[ ]:= lvgenuine["reactionsteps"]
Out[ ]= {A + X → 2 X, X + Y → 2 Y, Y → B}
In[ ]:= lv = ReactionsData[{"Lotka-Volterra"}, {"A", "B"}];
In[ ]:= lv["reactionsteps"]
Out[ ]= {A + X → 2 X, X + Y → 2 Y, Y → B}
In[ ]:= lv["fhjgraphedges"]
Out[ ]= {X → 2 X, X + Y → 2 Y, Y → 0}
```

```
lv["species"]
```

```
{X, Y}
```

```
lv["externalspecies"]
```

```
{A, B}
```

Constant pressure and volume; temperature may change. In- and outflow is represented using the empty complex.

Usual assumptions of the chemist (**mass conservation, low orders of reactions, reversibility, detailed balancing**) are not assumed from the beginning, they may be used as restrictions, their appearance can be checked using necessary and sufficient conditions, etc.

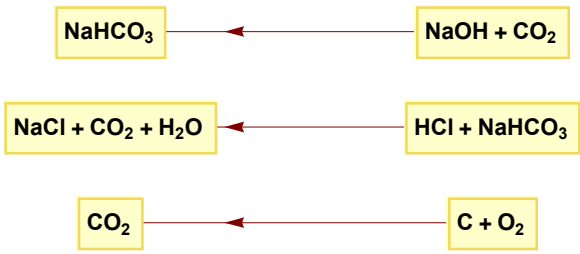
Graphs of reactions

Petri (13)

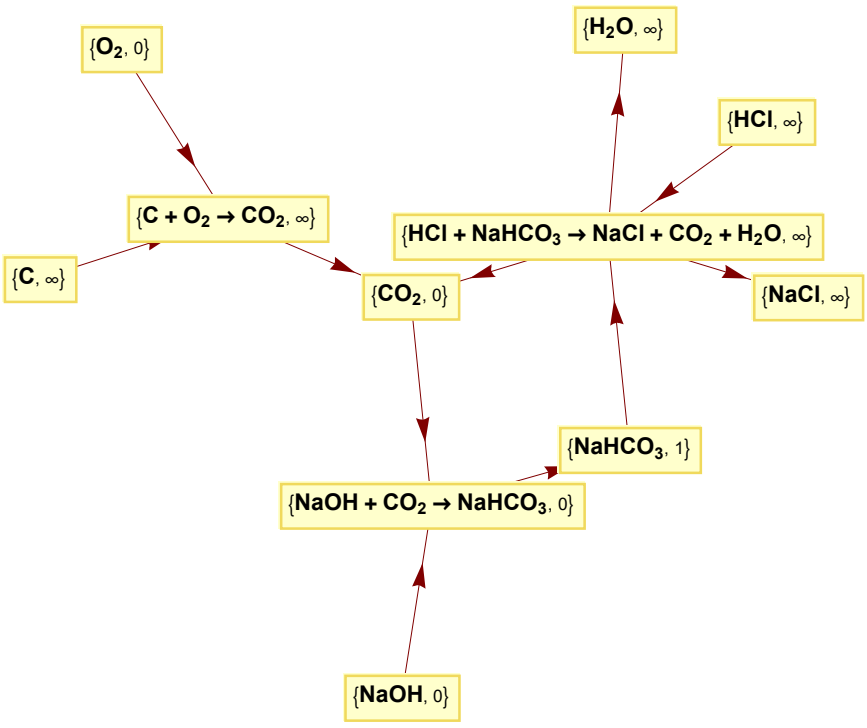
```
sm = ReactionsData[{"Petri"}]["species", "complexes", "reactionsteps"]
```

$$\{\{C, O_2, CO_2, NaOH, NaHCO_3, HCl, NaCl, H_2O\},$$
$$\{C + O_2, CO_2, NaOH + CO_2, NaHCO_3, HCl + NaHCO_3, NaCl + CO_2 + H_2O\},$$
$$\{C + O_2 \to CO_2, NaOH + CO_2 \to NaHCO_3, HCl + NaHCO_3 \to NaCl + CO_2 + H_2O\}\}$$

```
ShowFHJGraph[{"Petri"}, DirectedEdges → True, VertexLabeling → All,
  ImageSize → 300, Method -> "SpringEmbedding"] /. format[Flatten[sm], Bold, 12]
```

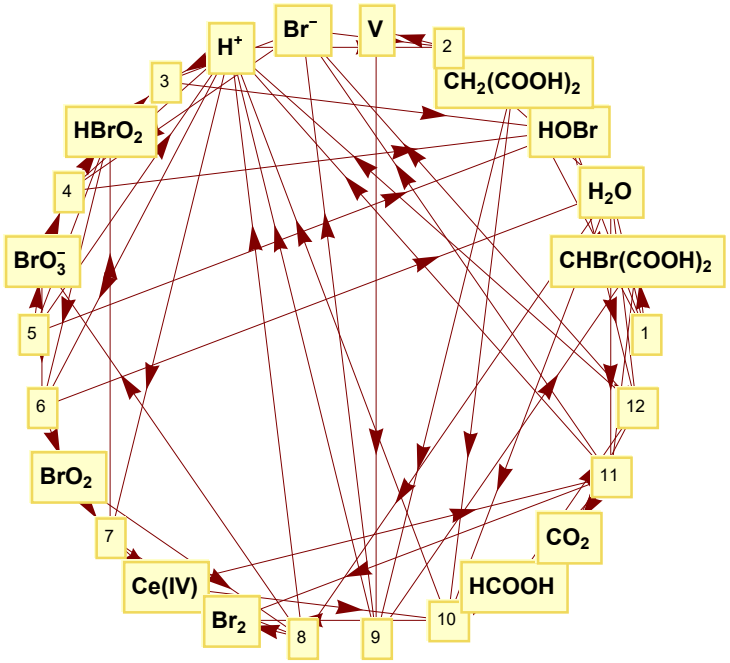



```
ShowVolpertGraph[{"Petri"}, DirectedEdges → True,
  VertexLabeling → All, ImageSize → 500, Method -> "SpringEmbedding",
  Indexed → {"CO2", "NaOH", "O2"}] /. format[Flatten[sm], Bold, 12]
```



Clarke

```
alias = {"A" → "CH2(COOH)2", "B" → "BrO3-", "H" → "H+",
    "M" → "CHBr(COOH)2", "P" → "HCOOH", "Q" → "CO2", "S" → "H2O", "T" → "HOBr",
    "U" → "BrO2", "W" → "Br2", "X" → "HBrO2", "Y" → "Br-", "Z" → "Ce(IV)"};
speccomp = Flatten[ReactionsData[{"Clarke"}]["species", "complexes"]] /. alias;
clarkeV = ShowVolpertGraph[GetReaction[{"Clarke"}] /. alias, DirectedEdges → True,
    VertexLabeling → True, EdgeLabeling → False, ImageSize → 400,
    Method → "CircularEmbedding", Numbered → True] /. format[speccomp, Bold, 12]
```



Acyclicity of the Volpert graph

has similar consequences as weak reversibility and zero deficiency together.

```
AcyclicGraphQ[Graph[{"X" → "Y", "X" + "Y" → "Z"}]]
```

```
True
```

```
AcyclicVolpertGraphQ[{"X" → "Y", "X" + "Y" → "Z"}]
```

```
True
```

MassConservation

$\exists\, \boldsymbol{\rho} > \mathbf{0} : \boldsymbol{\rho}^T(\boldsymbol{\beta} - \boldsymbol{\alpha}) = 0$

A reaction is mass conserving if and only if $\max_{\lambda,\boldsymbol{\rho}} \{\lambda;\ \boldsymbol{\rho}^T(\boldsymbol{\beta} - \boldsymbol{\alpha}) = 0,\ \boldsymbol{\rho} \geq \lambda .\mathbf{1},\ \boldsymbol{\rho}^T \mathbf{1} = 1\} > 0$.

```
MassConservationRelations[{"Lotka-Volterra"}]
```

$\{\rho_A > 0,\ \rho_X == \rho_A,\ \rho_Y == \rho_A,\ \rho_B == \rho_A\}$

```
MassConservationRelations[{"Lotka-Volterra"}, ExternalSpecies → {"A", "B"}]
```

```
False
```

Atoms conserved → mass conserved.

The methanol-formic acid esterification

```
AtomConservingQ[{"HCOOH" + "CH3OH" → "HCOOCH3" + "H2O"}]
```

```
{True}
```

```
ToAtomMatrix[{"HCOOH", "CH3OH", "HCOOCH3", "H2O"}, FormattedOutput → True, Frame → All]
```

Atoms\Molecules	HCOOH	CH3OH	HCOOCH3	H2O
C	1	1	2	0
H	2	4	4	2
O	2	1	2	1
charge	0	0	0	0

Decompositions

```
ElementaryReactions[{"H2", "O2", "H2O", "C", "O", "CO"}, 2]
```

$\{O2 \to 2\,O,\ H2O \to H2 + O,\ 2\,O \to O2,\ CO \to C + O,\ H2 + O2 \to H2O + O,\ H2 + O \to H2O,\ CO + H2 \to C + H2O,$
$C + O2 \to CO + O,\ C + H2O \to CO + H2,\ H2O + O \to H2 + O2,\ C + O \to CO,\ CO + O \to C + O2\}$

```
Decompositions[{"H" + "O2" + 3 "H2" → 3 "H" + 2 "H2O"},
 {"H" + "O2" → "O" + "OH", "O" + "H2" → "H" + "OH", "OH" + "H2" → "H" + "H2O",
  2 "H" → "H2", "H" + "OH" ⇔ "H2O"}, 10, Method → LPBased]
```

```
7 solution(s) found with 10 solved LPs.
```

$\{\{1, 1, 2, 0, 0, 0\}, \{1, 1, 3, 1, 0, 1\}, \{1, 1, 2, 0, 1, 1\},$
$\{1, 1, 4, 2, 0, 2\}, \{1, 1, 3, 1, 1, 2\}, \{1, 1, 2, 0, 2, 2\}, \{1, 1, 2, 0, 3, 3\}\}$

What is a kinetic differential equation?

```
DeterministicModel[{FHIII}, {k1, k-1, k2, k3, k4}, {x, y, z, t, u}][[1]] /. {w_[t] → w} //
 Column
```

$x' == y\,k_{-1} - x\,k_1 - x\,z\,k_2 + u\,y\,k_4$
$y' == -y\,k_{-1} + x\,k_1 + t\,k_3 - u\,y\,k_4$
$z' == -x\,z\,k_2 + u\,y\,k_4$
$t' == x\,z\,k_2 - t\,k_3$
$u' == t\,k_3 - u\,y\,k_4$

$\sum_{m=1}^{M} \alpha(m, r)\, X_m \to \sum_{m=1}^{M} \beta(m, r)\, X_m \quad (r = 1, 2, \ldots, R)$

$\dot{c}_m = \sum_{r=1}^{R} (\beta(m, r) - \alpha(m, r))\, k_r \prod_{p=1}^{M} {c_m}^{\alpha(p,r)}$, or shortly

$\dot{\boldsymbol{c}} = \boldsymbol{\gamma} \cdot \mathbf{diag}(\boldsymbol{k}) \cdot \boldsymbol{c}^{\boldsymbol{\alpha}} = \boldsymbol{P} \circ \boldsymbol{c}$

What it is not?

Genralized Lotka-Volterra model

$\dot{x}_m = x_m\left(\sum_{p=1}^{M} a_{mp}\, x_p + b_m\right)$

```
DeterministicModel[{3 "X" → 4 "X"}, {k}][[1]]
```

$\{c_X'[t] == k\, c_X[t]^3\}$

```
DeterministicModel[{"Robertson"}, {k1, k2, k3}, {a, b, c}][[1]] // Column
```

$a'[t] == -a[t]\, k_1 + b[t]\, c[t]\, k_3$

$b'[t] == a[t]\, k_1 - b[t]^2\, k_2 - b[t]\, c[t]\, k_3$

$c'[t] == b[t]^2\, k_2$

But: All the LV models are kinetic differential equations.

In[ ]:=
```
DeterministicModel[(antonov =
      {"X" ⇔ 2 "X", "Y" ⇔ 2 "Y", "Z" ⇔ 2 "Z", "X" + "Y" → 0, "Y" + "Z" → 0, "Z" + "X" → 0}),
   {1, 1, 1, 1, 1, 1, k1, k2, k3}, {x, y, z}][[1]] // Column
```

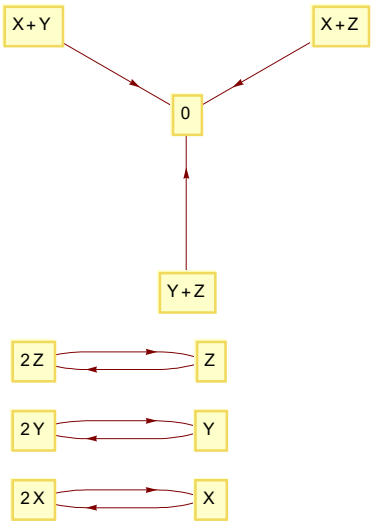
$x'[t] == x[t] - x[t]^2 - k_1\, x[t]\, y[t] - k_3\, x[t]\, z[t]$

Out[ ]= $y'[t] == y[t] - k_1\, x[t]\, y[t] - y[t]^2 - k_2\, y[t]\, z[t]$

$z'[t] == z[t] - k_3\, x[t]\, z[t] - k_2\, y[t]\, z[t] - z[t]^2$

In[ ]:=
```
ShowFHJGraph[{antonov}, DirectedEdges → True, VertexLabeling → All, ImageSize → 200]
```

Out[ ]=



Valery Antonov, Diana Dolicanin, Valery G. Romanovski, János Tóth: Invariant Planes and Periodic Oscillations in the May-Leonard Asymmetric Model, *MATCH Commun. Math. Comput. Chem.* **76** (2016) 455-474.

Kolmogorov systems

$\dot{x}_m = x_m f_m \circ \boldsymbol{x}$

See above, or

```
DeterministicModel[{"Brusselator"}, {a, 1, k1, b},
    {x, y}, ExternalSpecies → {"A", "B", "D", "E"}][[1]] // Column
```

$x'[t] == a - x[t] - b\,x[t] + k_1\,x[t]^2\,y[t]$

$y'[t] == x[t] - k_1\,x[t]^2\,y[t]$

However, here is a Kolmogorov system

```
DeterministicModel[
    {2 "X" + "Y" → 3 "X" + "Y", "X" + 2 "Y" → "X" + 3 "Y"}, {k1, k2}, {x, y}][[1]] // Column
```

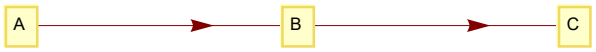
$x'[t] == k_1\,x[t]^2\,y[t]$

$y'[t] == k_2\,x[t]\,y[t]^2$

Monotone systems

$\dot{\boldsymbol{x}} = \boldsymbol{f} \circ \boldsymbol{x}$ $\boldsymbol{y}(0) \le \boldsymbol{z}(0)$ implies $\boldsymbol{y}(t) \le \boldsymbol{z}(t)$

```
ShowFHJGraph[{"Consecutive"}]
```



More generally (De Leenheer, Angeli, Sontag):

De Leenheer P., Angeli D., Sontag E. D. Monotone chemical reaction networks. *J. Math. Chem.* **41**(3) (2006), 295–314.

$\mathcal{C}_1 \Leftrightarrow \mathcal{C}_2 \Leftrightarrow \ldots \Leftrightarrow \mathcal{C}_{N-1} \Leftrightarrow \mathcal{C}_N$ (no common species in the complexes)

But in general, induced kinetic differential equations are not monotone systems.

In[ ]:=
```
re = ReactionsData[{"Lotka-Volterra"}, ExternalSpecies → {"A", "B"}]["fhjgraphedges"]
```

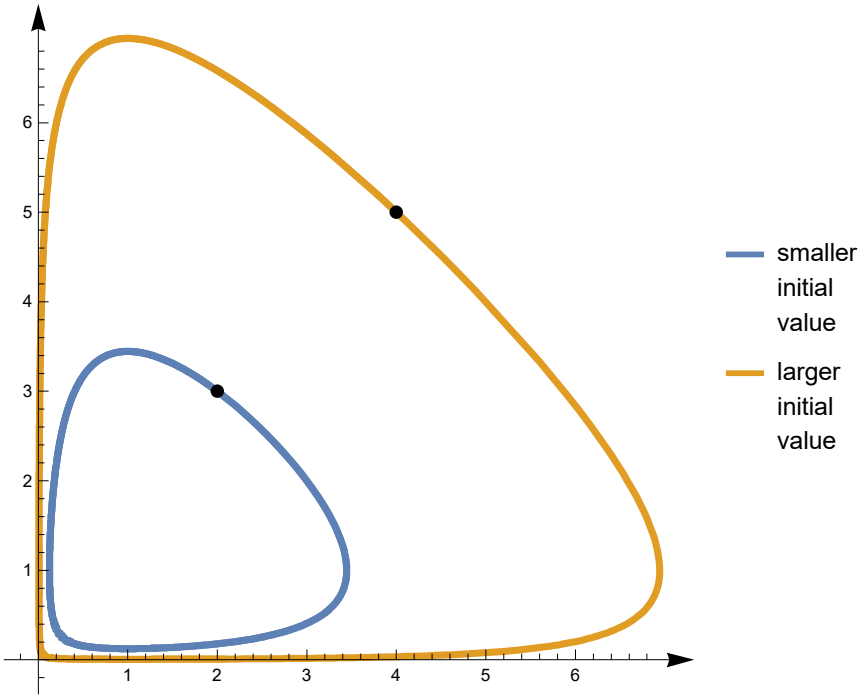
Out[ ]= $\{X \to 2\,X,\ X + Y \to 2\,Y,\ Y \to 0\}$

In[ ]:=
```
small = ReplaceAll @@ Concentrations[{re}, {1, 1, 1}, {2, 3}, {0, 20}, {x, y}];
```

In[ ]:=
```
large = ReplaceAll @@ Concentrations[{re}, {1, 1, 1}, {4, 5}, {0, 20}, {x, y}];
```

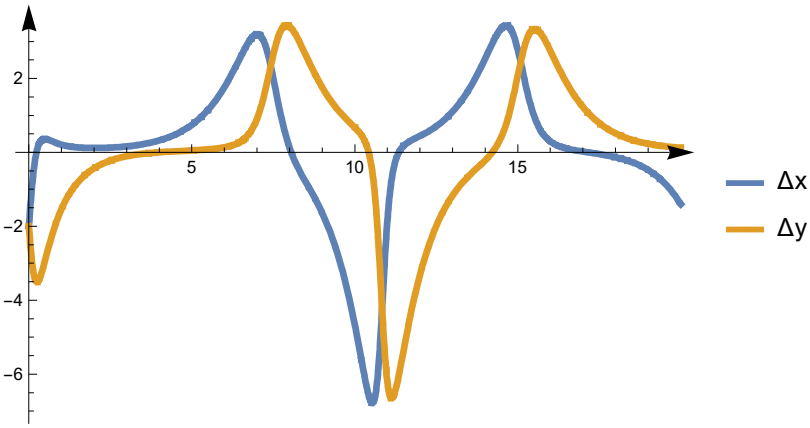
In[ ]:=
```
lvtwocurves1 = ParametricPlot[Evaluate[{small, large}],
  {t, 0, 20}, PlotRange -> All, PlotStyle → Directive[Thickness[0.01]],
  PlotLegends → {"smaller\ninitial\nvalue", "larger\ninitial\nvalue"},
  Epilog → {PointSize[Large], Point[{2, 3}], Point[{4, 5}]}]
```

Out[ ]=



In[ ]:=
```
lvtwocurves2 = Plot[Evaluate[{small - large}], {t, 0, 20}, PlotRange -> All,
  PlotStyle → Directive[Thickness[0.01]], PlotLegends → {"Δx", "Δy"}]
```

Out[ ]=



What it is?

A polynomial system without negative cross effect (Hárs-Tóth, 1979).

```
Column[{x' == y, y' == Framed[-x]}]
```

$$x' == y$$

$$y' == \boxed{-x}$$

```
Column[{x' == σ y - σ x, y' == ρ x - Framed[-x z], z' == x y - β z}]
```

$$x' == -x\,\sigma + y\,\sigma$$

$$y' == x\,\rho - \boxed{-x\,z}$$

$$z' == x\,y - z\,\beta$$

```
In[•]:= CrossEffectQ[polyval_, vars_] := Module[{M = Length[vars]},
          And @@ (Map[Not[Negative[#]] &, Flatten[MapThread[ReplaceAll,
                {MonomialList[polyval, vars],
                 Thread[vars → #] & /@ (1 - IdentityMatrix[M])}]]])]
```

```
In[•]:= CrossEffectQ[{y, -x}, {x, y}]
Out[•]= False
```

```
In[•]:= RightHandSide[{FHIII}, {k1, k-1, k2, k3, k4}, {x, y, z, t, u}]
```

$$\{y\,k_{-1} - x\,k_1 - x\,z\,k_2 + u\,y\,k_4,\ -y\,k_{-1} + x\,k_1 + t\,k_3 - u\,y\,k_4,\ -x\,z\,k_2 + u\,y\,k_4,\ x\,z\,k_2 - t\,k_3,\ t\,k_3 - u\,y\,k_4\}$$

```
In[•]:= CrossEffectQ[
         RightHandSide[{FHIII}, {k1, k-1, k2, k3, k4}, {x, y, z, t, u}], {x, y, z, t, u}]
Out[•]= ! Negative[k4] && ! Negative[k-1] && ! Negative[k1] &&
         ! Negative[k3] && ! Negative[k4] && ! Negative[k2] && ! Negative[k3]
```

In this talk we assume **mass action** type kinetics, thus rhs of other forms are excluded—although not in the program:

```
RightHandSide[{"H2" + "Br2" → 2 "HBr"},
 {k "H2" "Br2"^(3 / 2) / (K "HBr" + "Br2")}, MassAction → False]
```

$$\left\{-\frac{k\,c_{Br2}^{3/2}\,c_{H2}}{c_{Br2} + K\,c_{HBr}},\ -\frac{k\,c_{Br2}^{3/2}\,c_{H2}}{c_{Br2} + K\,c_{HBr}},\ \frac{2\,k\,c_{Br2}^{3/2}\,c_{H2}}{c_{Br2} + K\,c_{HBr}}\right\}$$

What is a polynomial? Homework: $f_m(\boldsymbol{x}) = \sum a_{\boldsymbol{k}}^m\,\boldsymbol{x}^{\boldsymbol{k}}$ if and only if the coordinate functions of $\boldsymbol{f}$ are univariate polynomials of all the variables. (Carroll, 1961.)

Equivalent forms

$$\dot{\boldsymbol{c}} = \boldsymbol{\gamma}\cdot\mathbf{diag}(\boldsymbol{k})\cdot\boldsymbol{c}^{\boldsymbol{\alpha}} = \boldsymbol{P}\circ\boldsymbol{c}$$

Network structure emphasized

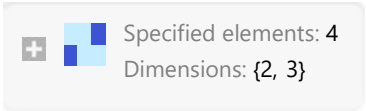
$\dot{c} = Y \cdot E \cdot \mathrm{diag}(k) \cdot c^{\alpha}$ (E is the **vertex-edge incidence matrix** of the reaction)

Lotka-Volterra:

```
ReactionsData[{"Lotka-Volterra"}, ExternalSpecies → {"A", "B"}]["complexes"]
```

```
{X, 2 X, X + Y, 2 Y, Y, 0}
```

```
α = ReactionsData[{"Lotka-Volterra"}, ExternalSpecies → {"A", "B"}]["α"]
```

```
SparseArray[ 

]
```

```
Y = ( 1 2 1 0 0 0
      0 0 1 2 1 0 ); E = ( -1  0  0
                            1  0  0
                            0 -1  0
                            0  1  0
                            0  0 -1
                            0  0  1 ); kk = ( k1
                                              k2
                                              k3 );
```

```
Y.E.(kk Times @@ {x, y}^α) // Flatten
```

```
{x k1 - x y k2, x y k2 - y k3}
```

```
RightHandSide[{"Lotka-Volterra"}, {k1, k2, k3}, {x, y}, ExternalSpecies → {"A", "B"}]
```

```
{x k1 - x y k2, x y k2 - y k3}
```

How to find the incidence matrix? Use the function IncidenceMatrix ☺

```
lot = Graph[ReactionsData[{"Lotka-Volterra"}]["fhjgraphedges"]];
TableForm[IncidenceMatrix[#],
    TableHeadings → {VertexList[#], EdgeList[#]}, TableAlignments → Right] &[lot]
```

	A + X ⟷ 2 X	X + Y ⟷ 2 Y	Y ⟷ B
A + X	−1	0	0
2 X	1	0	0
X + Y	0	−1	0
2 Y	0	1	0
Y	0	0	−1
B	0	0	1

Linearity in the reaction rate coefficients emphasized

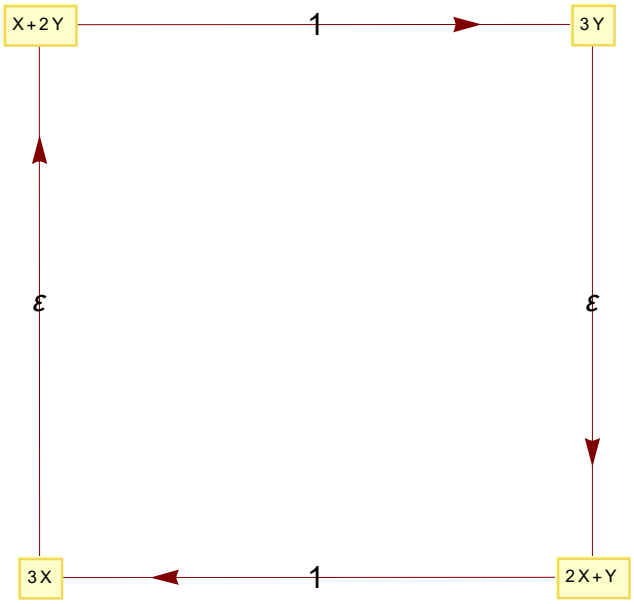
$\dot{c} = y \cdot \mathrm{diag}(c^{\alpha}) \cdot k$

Stationary points

Existence, uniqueness

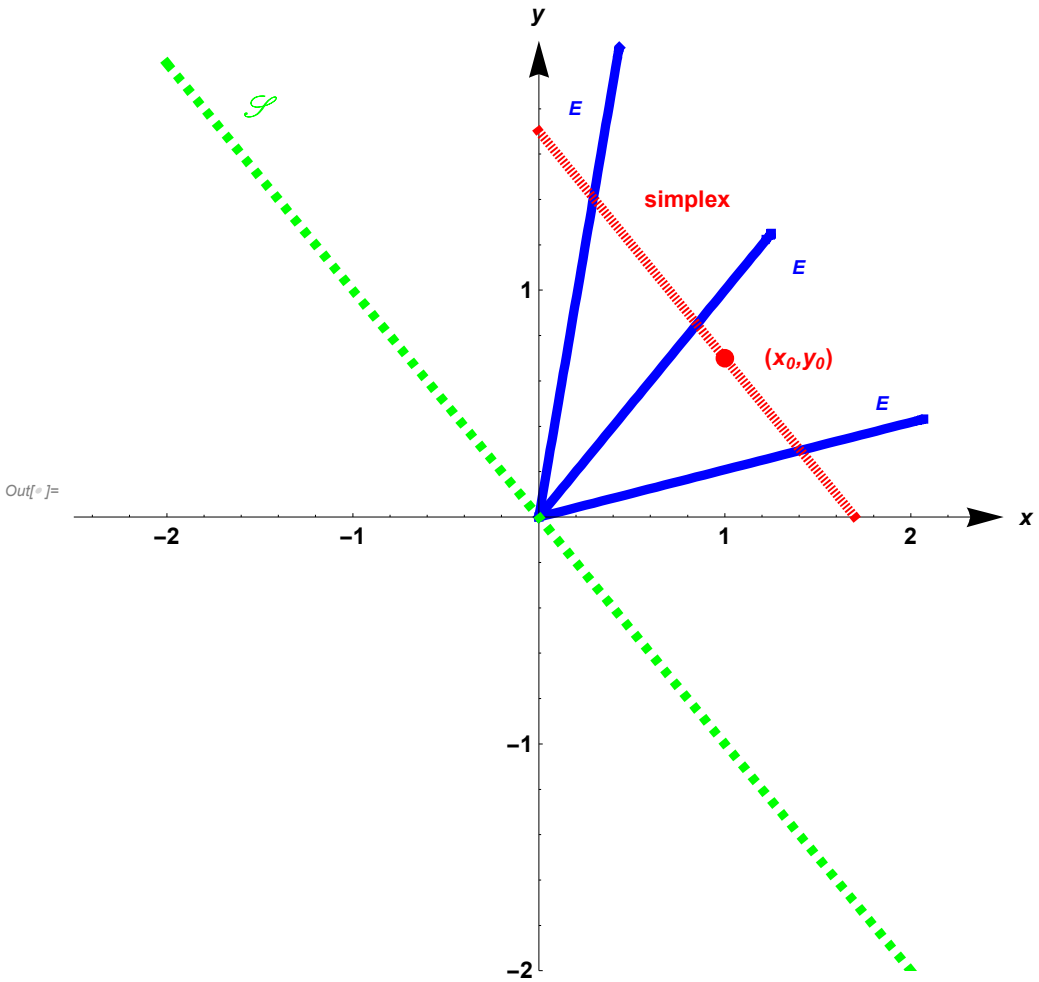
In[ ]:=
```
hjreaction = ShowFHJGraph[
  {2 "X" + "Y" → 3 "X", 3 "X" → "X" + 2 "Y", "X" + 2 "Y" → 3 "Y", 3 "Y" → 2 "X" + "Y"},
  {Style[1, 16], Style[ε, 16], Style[1, 16], Style[ε, 16]},
  DirectedEdges → True, VertexLabeling → All, Method → "SpringEmbedding"]
```

Out[ ]=



In[ ]:=
```
ClearAll[statcurves, m, n, u, a, b, ϵ, x, y];
statcurves[u_] := PowerExpand[{x, y} /. Cases[
      Last[Simplify[StationaryPoints[{"Horn-Jackson"}, {ϵ, 1, ϵ, 1}, {m, n}, {x, y}],
        Assumptions → (0 < ϵ < 1/6)]], {a_?TrueQ, b___} → {b}] /. m → (u - n) /. ϵ → 1 / 12]
hornjackson = ParametricPlot[Evaluate[statcurves[u]], {u, 0, 2.5},
  PlotStyle → Directive[{Blue, Thickness[0.01]}], AspectRatio → 1,
  Epilog → {Dashed, Green, Thickness[0.01], Line[{{-2, 2}, {2, -2}}], Dashing[{0}],
    Red, Thickness[0.01], Line[{{0, 1.7}, {1.7, 0}}], PointSize[0.02],
    Point[{1.0, 0.7}], Text[Style["(x0,y0)", Italic, Bold, 12], {1.4, 0.7}],
    Green, Text[Style["S", FontFamily → "Kunstler Script", Bold, 16], {-1.5, 1.8}],
    Red, Text[Style["simplex", Bold, 12], {0.8, 1.4}], Blue,
    Text[Style["E", Italic, Bold, 10], {1.85, 0.5}], Text[Style["E", Italic, Bold, 10],
     {1.4, 1.1}], Text[Style["E", Italic, Bold, 10], {0.2, 1.8}]},
  PlotRange → {{-2.5, 2.5}, {-2.0, 2.1}}, AxesLabel →
   (Style[#, Bold, Italic, 12] & /@ {"x", "y"}),
  TicksStyle → Directive[Black, Bold, 12], ImageSize → 500]
```

Out[ ]=



Weak reversibility does not imply uniqueness. However,

Weak reversibility implies existence of stationary points in all positive stoichiometric compatibility classes (Boros, 2017).

Absolute Concentration Robustness

```
StationaryPoints[{"X" + "Y" → 2 "Y", "Y" → "X"}, {k1, k2}, {x0, y0}][[2, 1]]
```

$$\left\{k_1 > \frac{k_2}{x_0 + y_0},\ c_X^* \to \frac{k_2}{k_1},\ c_Y^* \to \frac{-k_2 + k_1 x_0 + k_1 y_0}{k_1}\right\}$$

Now matter what the stationary concentration is, the first component does not depend on the initial concentrations: A kind of stability, may be useful from biological point of view. (Feinberg, Shinar).

```
AbsoluteConcentrationRobustness[{"X" + "Y" → 2 "Y", "Y" → "X"}]
```

```
{X}
```

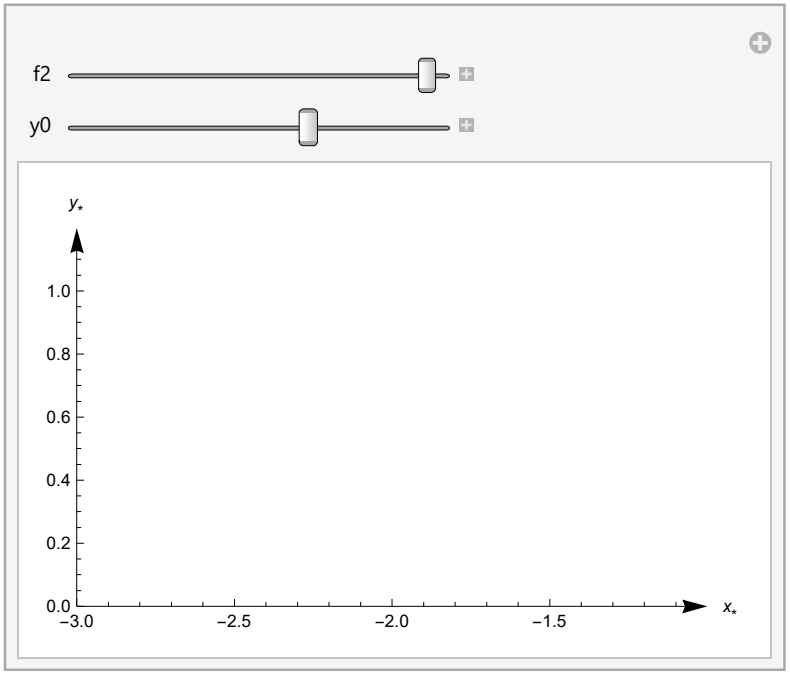
Also in the stochastic model.

Parameter dependence

```
x' = -x y + f (1 - x)
y' = x y + y ((1 - f2/f) y0 - y) + (f - f2) y0 - f y
```

In[ ]:=
```
lilipota[f2_, y0_, f_] := f x^3 - f x^2 + x (f^2 + (f - f2) y0) - f^2;
Manipulate[
 ParametricPlot[(XX[f2_, y0_, j_] := x /. NSolve[lilipota[f2, y0, 10^j] == 0, {x}];
   Distribute[{j, XX[f2, y0, j]}, List]), {j, -3, -1},
  PlotRange → {{-3, -1}, {0, 1.2}}, AxesLabel → {"x*", "y*"}],
 {{f2, 1/135}, 0.0009, 0.0075, 0.0001}, {{y0, 10/27}, 0.24, 0.38, 0.01}]
```

Out[ ]=



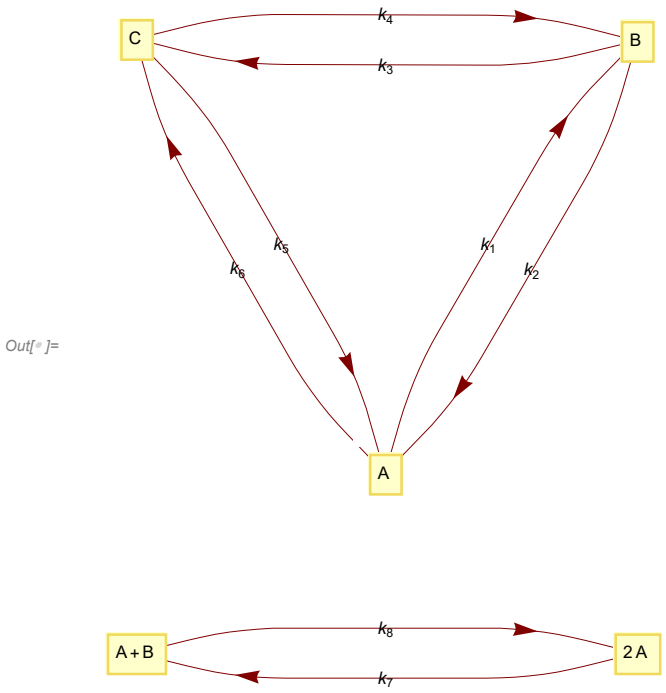
Detailed balance

A reaction only consisting of reversible steps is detailed balanced at the positive stationary concentration $\boldsymbol{c}_*$, if for all steps $k_p \boldsymbol{c}_*^{\alpha(\cdot,p)} = k_{-p} \boldsymbol{c}_*^{\beta(\cdot,p)}$ holds. (Conditions: Feinberg; Fredholm)

Nagy, I., Tóth, J.: Microscopic reversibility or detailed balance in ion channel models. *J. Math. Chem.* **50** (5) (2012), 1179–1199.
Nagy, I., Kovács, B., Tóth, J.: Detailed balance in ion channels: Applications of Feinberg' s theorem. *React. Kinet. Catal. Lett.* **96** (2) (2009), 263–267.

In[ ]:=
```
ShowFHJGraph[
 complicated = Join[GetReaction[{"Wegscheider"}], ToReversible["Triangle"]],
 {k1, k2, k7, k8, k3, k4, k5, k6}, EdgeLabeled → True]
```

Out[ ]=




```
DetailedBalanced[complicated, {k1, k2, k7, k8, k3, k4, k5, k6}]
```

$\{k_2\, k_4\, k_6 == k_1\, k_3\, k_5,\ k_2\, k_7 == k_1\, k_8\}$

Tóth, J.; Nagy, A. L.; Zsély, I. Gy.: Structural analysis of combustion mechanisms, *J. Math. Chem.* **53** (2015), 86–110.

In a mechanism for hydrogen combustion (9 species, 7 independent rection steps,
$\delta = 41 - 16 - 7 = 18$,) given by Starik et al. (2009)

A.M. Starik, N.S. Titova, A.S. Sharipov, V.E. Kozlov: Syngas oxidation mechanism. *Combust. Explos. Shock Waves* **46**(5) (2010), 491–506.

$$\{k_2 k_4 k_5 == k_1 k_3 k_6,\ k_3 k_8 k_{11} == k_4 k_7 k_{12},\ k_2 k_{14} k_{19} == k_1 k_{13} k_{20},$$
$$k_4 k_{28} k_{31} == k_3 k_{27} k_{32},\ k_4 k_{13} k_{41} == k_3 k_{14} k_{42},\ k_{18} k_{21} k_{32} == k_{17} k_{22} k_{31},$$
$$k_2 k_9 k_{14} k_{15} == k_1 k_{10} k_{13} k_{16},\ k_2 k_8 k_9 k_{21} == k_1 k_7 k_{10} k_{22},\ k_2 k_4 k_9 k_{23} == k_1 k_3 k_{10} k_{24},$$
$$k_2 k_4 k_{30} k_{31} == k_1 k_3 k_{29} k_{32},\ k_3 k_{14} k_{32} k_{35} == k_4 k_{13} k_{31} k_{36},\ k_1 k_3 k_{10} k_{32} k_{33} == k_2 k_4 k_9 k_{31} k_{34},$$
$$k_3 k_{14} k_{32} k_{38} k_{43} == k_4 k_{13} k_{31} k_{37} k_{44},\ k_2 k_4^2 k_8 k_9 k_{13} k_{26} k_{31}^2 == k_1 k_3^2 k_7 k_{10} k_{14} k_{25} k_{32}^2,$$
$$k_2 k_4 k_8 k_9 k_{13} k_{31} k_{39} == k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{40},\ k_4 k_8 k_9 k_{13}^2 k_{31} k_{37} k_{49} == k_3 k_7 k_{10} k_{14}^2 k_{32} k_{38} k_{50},$$
$$k_2 k_4 k_8 k_9 k_{31} k_{37} k_{51} == k_1 k_3 k_7 k_{10} k_{32} k_{38} k_{52},\ k_1 k_3^2 k_7 k_{10} k_{14} k_{32}^2 k_{38} k_{45} == k_2 k_4^2 k_8 k_9 k_{13} k_{31}^2 k_{37} k_{46},$$
$$k_2 k_4 k_8 k_9 k_{13} k_{31} k_{37} k_{47} == k_1 k_3 k_7 k_{10} k_{14} k_{32} k_{38} k_{48}\}$$

Carbon monoxide, methanol: more complicated.

First integrals

Nagy, I., Tóth, J.: Quadratic first integrals of kinetic differential equations. *J. Math. Chem.* **52**(1) (2014) , 93–114.

Numerics

Stiff equations

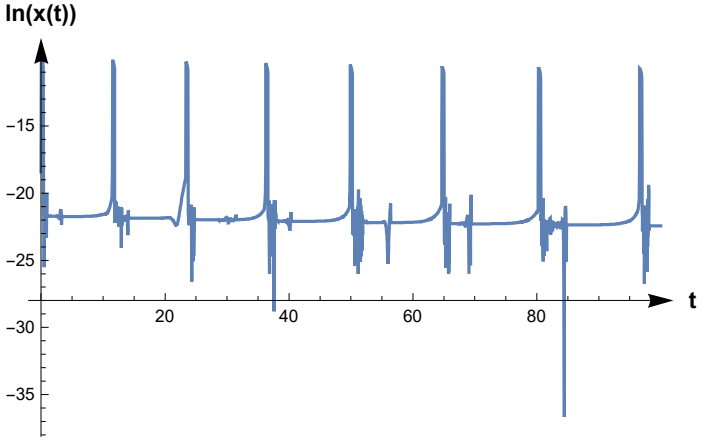
Taken from the book by Deuflhard and Bornemann who give the reaction rate coefficients (pp. 17--18), but no concentrations, still one can reproduce their results quite well.

Oregonator - the role of options

```
In[•]:= ClearAll[a, y, x, p];
        or = GetReaction["Oregonator"] /. {fOregonator → 1} /. {"B" → "A", "Q" → "P"}
Out[•]= {A + Y → X, X + Y → P, A + X → 2 X + Z, 2 X → P, Z → Y}

In[•]:= cin = Concentrations[{or}, {134 / 100, 16 × 10^8, 8 × 10^3, 4 × 10^7, 1},
          {5 × 10^-1, 10^-6, 10^-8, 6 × 10^-2, 10^-4}, {0, 100}, {a, y, x, p, z}];
        bzdeuflhardA = Plot[Log[x[t] /. Last[cin]], {t, 0, 100}, PlotRange → All,
          AxesLabel → (Style[#, Bold, 12] & /@ {"t", "ln(x(t))"}), AxesOrigin → {0, -28}]
```

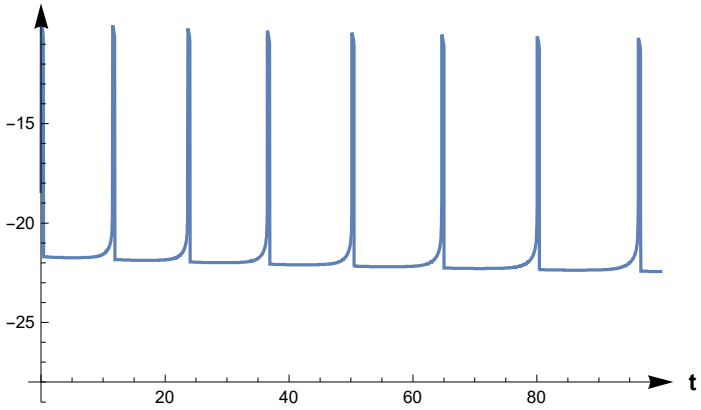
Out[•]=



In[ ]:=
```
con = Concentrations[{or}, {134 / 100, 16 × 10^8, 8 × 10^3, 4 × 10^7, 1},
    {5 × 10^-1, 10^-6, 10^-8, 6 × 10^-2, 10^-4}, {0, 100}, {a, y, x, p, z},
    Method → "BDF", WorkingPrecision → 32, MaxSteps → 10^6];
bzdeuflhardB = Plot[Log[x[t] /. Last[con]], {t, 0, 100}, PlotRange → All,
  AxesLabel → (Style[#, Bold, 12] & /@ {"t", "ln(x(t))"}), AxesOrigin → {0, -28}]
```

ln(x(t))

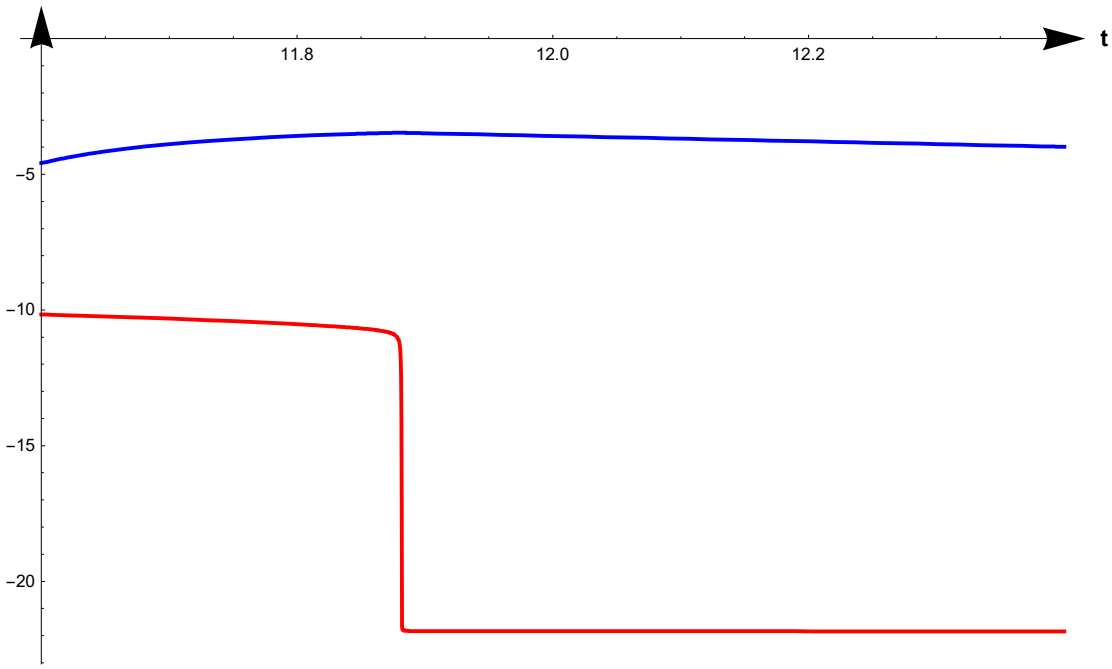
Out[ ]=



In[ ]:=
```
bzdeuflhardStiff = Plot[Evaluate[Log[{x[t], z[t]} /. Last[con]]],
  {t, 11.6, 12.4}, PlotStyle → {Directive[Thick, Red], Directive[Thick, Blue]},
  AxesLabel → {Style["t", Bold, 12],
    Row[{Style["(", Bold, 12], Style["ln(x(t))", Red, Bold, 12], Style[", ", Bold, 12],
      Style["ln(z(t))", Blue, Bold, 12], Style[")", Bold, 12]}]}, ImageSize → 600]
```

(ln(x(t)), ln(z(t)))

Out[ ]=

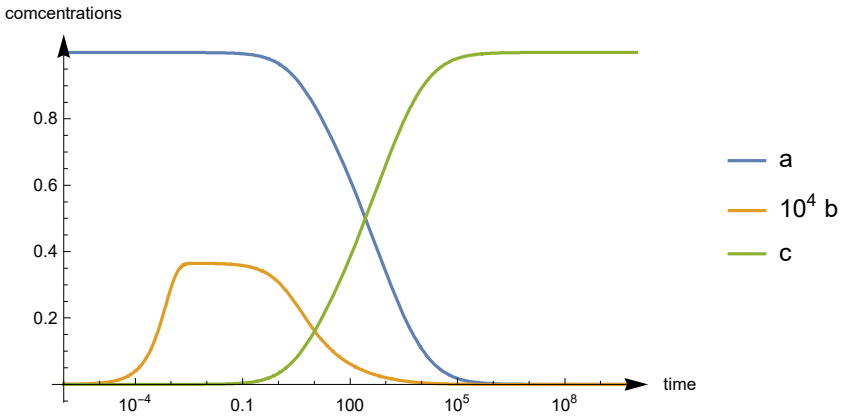


Robertson - as ODE, as DAE

ODE

In[ ]:=
```
conrob = Concentrations[{rob = GetReaction["Robertson"]},
    {0.04, 3 × 10^7, 10^4}, {1, 0, 0}, {0, 10^10}];
robertsonexact = LogLinearPlot[Evaluate[{1, 10^4, 1} (ReplaceAll @@ conrob)],
  {t, 10^-6, 10^10}, PlotLegends → {"a", "10^4 b", "c"},
  PlotRange → All, AxesLabel → {"time", "comcentrations"}]
```

Out[ ]=



Why is it interesting (“a challenge”)?

```
dm = DeterministicModel[{rob}, {0.04, 3 × 10^7, 10^4}, {a, b, c}]
```

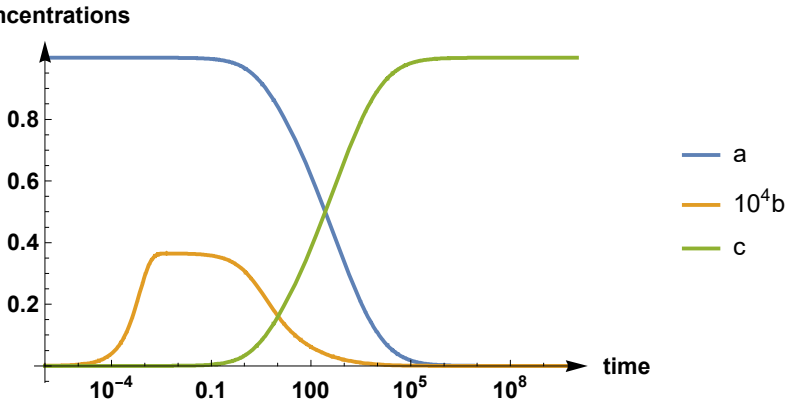
$$\{\{a'[t] == -0.04\, a[t] + 10\,000\, b[t]\, c[t],\ b'[t] == 0.04\, a[t] - 30\,000\,000\, b[t]^2 - 10\,000\, b[t]\, c[t],\ c'[t] == 30\,000\,000\, b[t]^2\},\ \{a[t], b[t], c[t]\}\}$$

DAE

In[ ]:=
```
nds = NDSolve[{a'[t] == -0.04` a[t] + 10 000 b[t] c[t], a[t] + b[t] + c[t] == 1,
    c'[t] == 30 000 000 b[t]^2, a[0] == 1, c[0] == 0}, {a[t], b[t], c[t]}, {t, 10^-6, 10^10}];
```

```
In[ ]:= robertsonDAE = LogLinearPlot[Evaluate[{1, 10^4, 1} {a[t], b[t], c[t]} /. nds],
          {t, 10^-6, 10^10}, PlotLegends → {"a", "10^4b", "c"}, PlotRange → All,
          PlotStyle → Thick, AxesLabel → (Style[#, 12, Bold] & /@ {"time", "comcentrations"}),
          TicksStyle → Directive[Black, Bold, 12]]
```

Out[ ]=



Quite similar to the exact figure.

Can you find the stationary point?

```
rhs = RightHandSide[{0 → X1 ⇔ X2 ⇔ X3 ⇔ X4 ⇔ X5 ⇔ X6 ⇔ X7 ⇔ X8 → 0}, Join[{k0},
    Flatten[Transpose[{k# & /@ Range[7], k# & /@ -Range[7]}]], {k8}], x# & /@ Range[8]]
```

We can only verify it:

```
rhs /. {xi_ → k0 Sum[Product[k1, {l, 10 - j, 8}]
        Product[k-1, {l, i, 8 - j}] / Product[k1, {l, i, 8}], {j, 1, 9 - i}]} // Simplify
```

It works in simple cases :)

```
StationaryPoints[{2 "X" ⇔ "Y"}, {κ, λ}, {x0, y0}] // PowerExpand
```

Out[ ]=

$$\left\{\left\{c_X^*,\ c_Y^*\right\},\ \left\{\left\{c_X^* \to -\frac{1}{4\,\kappa}\left(\lambda - \sqrt{\lambda}\ \sqrt{8\,x0\,\kappa + 16\,y0\,\kappa + \lambda}\right),\right.\right.\right.$$
$$\left.\left.\left.c_Y^* \to \frac{1}{8\,\kappa}\left(4\,x0\,\kappa + 8\,y0\,\kappa + \lambda - \sqrt{\lambda}\ \sqrt{8\,x0\,\kappa + 16\,y0\,\kappa + \lambda}\right)\right\}\right\}\right\}$$

Good numerical methods

The Euler method when applied with a small enough step size keeps the invariance of the first orthant.
The stationary points of an autonomous differential equation are the same as those obtained by the Euler method.

Stochastic model

Symbolic calculations (limited:))

In[]:=
```
gene = {"inactive gene" ⇔ "active gene" → "messenger" → "protein" → 0, "messenger" → 0};
```

In[]:=
```
ClearAll[i, a, m, p, G];
MasterEquation[{gene}, {λ1, λ-1, λ2, λ3, γ+, γ-}, {t, i, a, m, p}, P]
```

Out[]=
$$\{P^{(1,0,0,0,0)}[t, i, a, m, p] == (1+m)\,P[t, i, a, 1+m, p]\,\gamma_- + (1+p)\,P[t, i, a, m, 1+p]\,\gamma_+ + (1+a)\,P[t, -1+i, 1+a, m, p]\,\lambda_{-1} + (1+i)\,P[t, 1+i, -1+a, m, p]\,\lambda_1 + (1+a)\,P[t, i, 1+a, -1+m, p]\,\lambda_2 + (1+m)\,P[t, i, a, 1+m, -1+p]\,\lambda_3 - P[t, i, a, m, p]\,(m\,\gamma_- + p\,\gamma_+ + a\,\lambda_{-1} + i\,\lambda_1 + a\,\lambda_2 + m\,\lambda_3)\}$$

In[]:=
```
ProbabilityGeneratingFunctionEquation[
 {gene}, {λ1, λ-1, λ2, λ3, γ+, γ-}, {t, x, y, u, v}, G]
```

Out[]=
$$G^{(1,0,0,0,0)}[t, x, y, u, v] == (1-v)\,\gamma_+\,G^{(0,0,0,0,1)}[t, x, y, u, v] + (1-u)\,\gamma_-\,G^{(0,0,0,1,0)}[t, x, y, u, v] + (-u+v)\,\lambda_3\,G^{(0,0,0,1,0)}[t, x, y, u, v] + (x-y)\,\lambda_{-1}\,G^{(0,0,1,0,0)}[t, x, y, u, v] + (u-y)\,\lambda_2\,G^{(0,0,1,0,0)}[t, x, y, u, v] + (-x+y)\,\lambda_1\,G^{(0,1,0,0,0)}[t, x, y, u, v]$$

In[]:=
```
SolveProbabilityGeneratingFunctionEquation[{gene}, {λ1, λ-1, λ2, λ3, γ+, γ-},
 {1, 0, 0, 0}, {t, x, y, u, v}, G, Method → "MatrixExponential"]
```

SolveProbabilityGeneratingFunctionEquation: The order of the reaction is at most one, thus the method "Characteristics" can also be applied.

Out[]=
$$\{G[t, x, y, u, v],$$

$$G[t, x, y, u, v] \to 1 + (-1+u)\left(\left(e^{t\,(-\gamma_- - \lambda_3)}\,\lambda_2\,(\gamma_-\,\lambda_1 - \gamma_+\,\lambda_1 + \lambda_1\,\lambda_3)\right) \Big/ \left((\gamma_- - \gamma_+ + \lambda_3)\left(\gamma_-^2 - \gamma_-\,\lambda_{-1} - \gamma_-\,\lambda_1 - \gamma_-\,\lambda_2 + \lambda_1\,\lambda_2 + 2\,\gamma_-\,\lambda_3 - \lambda_{-1}\,\lambda_3 - \lambda_1\,\lambda_3 - \lambda_2\,\lambda_3 + \lambda_3^2\right)\right) - \left(e^{\frac{1}{2}t\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2}\right)}\,\lambda_2\left(-2\,\gamma_+\,\lambda_1 + \lambda_{-1}\,\lambda_1 + \lambda_1^2 + \lambda_1\,\lambda_2 + \lambda_1\sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)\right) \Big/ \left(2\left(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 + \gamma_-\,\lambda_1\,\lambda_2 + \gamma_+\,\lambda_1\,\lambda_2 + \frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 + \gamma_+\,\lambda_1\,\lambda_3 + \gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^2 (3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) + \frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)(2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} + 2\,\gamma_-\,\lambda_1 + 2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 + 2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3)\right)\right) - \left(e^{\frac{1}{2}t\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2}\right)}\,\lambda_2\left(-2\,\gamma_+\,\lambda_1 + \lambda_{-1}\,\lambda_1 + \lambda_1^2 + \lambda_1\,\lambda_2 -\right.\right.$$

$$\lambda_1 \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\Big)\Big/\Big(2\Big(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 + \gamma_-\,\lambda_1\,\lambda_2 +$$

$$\gamma_+\,\lambda_1\,\lambda_2 + \frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 +$$

$$\gamma_+\,\lambda_1\,\lambda_3 + \gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^2$$

$$(3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) +$$

$$\frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)(2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} + 2\,\gamma_-$$

$$\lambda_1 + 2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 + 2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3)\Big)\Big)\Big) +$$

$$(-1+v)\left(-\left(\left(e^{-t\,\gamma_+}\,\lambda_1\,\lambda_2\,\lambda_3\right)\Big/\left(\left(\gamma_+^2 - \gamma_+\,\lambda_{-1} - \gamma_+\,\lambda_1 - \gamma_+\,\lambda_2 + \lambda_1\,\lambda_2\right)(-\gamma_- + \gamma_+ - \lambda_3)\right)\right) -\right.$$

$$\left(e^{t\,(-\gamma_- - \lambda_3)}\,\lambda_1\,\lambda_2\,\lambda_3\right)\Big/$$

$$\left((\gamma_- - \gamma_+ + \lambda_3)\left(\gamma_-^2 - \gamma_-\,\lambda_{-1} - \gamma_-\,\lambda_1 - \gamma_-\,\lambda_2 + \lambda_1\,\lambda_2 + 2\,\gamma_-\,\lambda_3 - \lambda_{-1}\,\lambda_3 - \lambda_1\,\lambda_3 - \lambda_2\,\lambda_3 + \lambda_3^2\right)\right) +$$

$$\left(e^{\frac{1}{2}t\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2}\right)}\,\lambda_1\,\lambda_2\,\lambda_3\right)\Big/$$

$$\Big(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 + \gamma_-\,\lambda_1\,\lambda_2 + \gamma_+\,\lambda_1\,\lambda_2 +$$

$$\frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 + \gamma_+\,\lambda_1\,\lambda_3 +$$

$$\gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^2$$

$$(3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) +$$

$$\frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)(2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} +$$

$$2\,\gamma_-\,\lambda_1 + 2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 + 2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3)\Big) +$$

$$\left(e^{\frac{1}{2}t\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2}\right)}\,\lambda_1\,\lambda_2\,\lambda_3\right)\Big/\Big(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 +$$

$$\gamma_-\,\lambda_1\,\lambda_2 + \gamma_+\,\lambda_1\,\lambda_2 + \frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 +$$

$$\gamma_+\,\lambda_1\,\lambda_3 + \gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)^2$$

$$(3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) +$$

$$\frac{1}{2}\left(-\lambda_{-1}-\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)(2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} + 2\,\gamma_-\,\lambda_1 +$$

$$2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 + 2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3)\Big)\Big) + (-1+x)$$

$$\left(-\left(\left(e^{t\,(-\gamma_- - \lambda_3)}\left(\lambda_{-1}\left((\gamma_+ - \lambda_1)\,\lambda_1 + \frac{1}{2}\lambda_1\left(-\lambda_{-1}+\lambda_1-\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)\right) +\right.\right.\right.$$

$$\frac{1}{2}\left(\lambda_{-1}-\lambda_1+\lambda_2-\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)$$

$$\left.\left.\left.\left(\lambda_{-1}\,\lambda_1 + \frac{1}{2}(\gamma_+ - \lambda_1)\left(\lambda_{-1}-\lambda_1+\lambda_2+\sqrt{\left(-4\,\lambda_1\,\lambda_2+(\lambda_{-1}+\lambda_1+\lambda_2)^2\right)}\right)\right)\right)\right)\Big/$$

$$\left((\gamma_- - \gamma_+ + \lambda_3) \left(\gamma_-^2 - \gamma_- \lambda_{-1} - \gamma_- \lambda_1 - \gamma_- \lambda_2 + \lambda_1 \lambda_2 + 2 \gamma_- \lambda_3 - \lambda_{-1} \lambda_3 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2 \right) \right) -$$

$$\left(e^{-t \gamma_+} \left(\lambda_{-1} \left(\frac{1}{2} \lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) + \right. \right. \right.$$

$$\left. \left. \frac{1}{2} \lambda_1 \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) +$$

$$\left(\lambda_{-1} \lambda_1 + \frac{1}{4} \left(\lambda_{-1} - \lambda_1 + \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right.$$

$$\left. \left. \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) (\gamma_- - \lambda_1 + \lambda_3) \right) \Big/$$

$$\left(\left(\gamma_+^2 - \gamma_+ \lambda_{-1} - \gamma_+ \lambda_1 - \gamma_+ \lambda_2 + \lambda_1 \lambda_2 \right) (-\gamma_- + \gamma_+ - \lambda_3) \right) + \left(e^{\frac{1}{2} t \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2} \right)} \right.$$

$$\left(\lambda_{-1} \left((\gamma_+ - \lambda_1) \lambda_1 + \frac{1}{2} \lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) + \right.$$

$$\left(\lambda_{-1} \lambda_1 + \frac{1}{2} (\gamma_+ - \lambda_1) \left(\lambda_{-1} - \lambda_1 + \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right)$$

$$\left. (\gamma_- - \lambda_1 + \lambda_3) \right) \Big/ \left(\gamma_- \gamma_+ \lambda_{-1} + \gamma_- \gamma_+ \lambda_1 + \gamma_- \gamma_+ \lambda_2 + \gamma_- \lambda_1 \lambda_2 + \gamma_+ \lambda_1 \lambda_2 + \right.$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^3 + \gamma_+ \lambda_{-1} \lambda_3 + \gamma_+ \lambda_1 \lambda_3 +$$

$$\gamma_+ \lambda_2 \lambda_3 + \lambda_1 \lambda_2 \lambda_3 + \frac{1}{4} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^2$$

$$(3 \gamma_- + 3 \gamma_+ + 3 \lambda_{-1} + 3 \lambda_1 + 3 \lambda_2 + 3 \lambda_3) +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)$$

$$(2 \gamma_- \gamma_+ + 2 \gamma_- \lambda_{-1} + 2 \gamma_+ \lambda_{-1} + 2 \gamma_- \lambda_1 + 2 \gamma_+ \lambda_1 + 2 \gamma_- \lambda_2 + 2 \gamma_+ \lambda_2 + 2 \lambda_1 \lambda_2 +$$

$$\left. 2 \gamma_+ \lambda_3 + 2 \lambda_{-1} \lambda_3 + 2 \lambda_1 \lambda_3 + 2 \lambda_2 \lambda_3) \right) + \left(e^{\frac{1}{2} t \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2} \right)} \right.$$

$$\left(\lambda_{-1} \left((\gamma_+ - \lambda_1) \lambda_1 + \frac{1}{2} \lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) + \right.$$

$$\left(\lambda_{-1} \lambda_1 + \frac{1}{2} (\gamma_+ - \lambda_1) \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right)$$

$$\left. (\gamma_- - \lambda_1 + \lambda_3) \right) \Big/ \left(\gamma_- \gamma_+ \lambda_{-1} + \gamma_- \gamma_+ \lambda_1 + \gamma_- \gamma_+ \lambda_2 + \gamma_- \lambda_1 \lambda_2 + \gamma_+ \lambda_1 \lambda_2 + \right.$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^3 + \gamma_+ \lambda_{-1} \lambda_3 + \gamma_+ \lambda_1 \lambda_3 +$$

$$\gamma_+ \lambda_2 \lambda_3 + \lambda_1 \lambda_2 \lambda_3 + \frac{1}{4} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^2$$

$$(3 \gamma_- + 3 \gamma_+ + 3 \lambda_{-1} + 3 \lambda_1 + 3 \lambda_2 + 3 \lambda_3) +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) (2 \gamma_- \gamma_+ + 2 \gamma_- \lambda_{-1} + 2 \gamma_+ \lambda_{-1} +$$

$$\left. 2 \gamma_- \lambda_1 + 2 \gamma_+ \lambda_1 + 2 \gamma_- \lambda_2 + 2 \gamma_+ \lambda_2 + 2 \lambda_1 \lambda_2 + 2 \gamma_+ \lambda_3 + 2 \lambda_{-1} \lambda_3 + 2 \lambda_1 \lambda_3 + 2 \lambda_2 \lambda_3) \right) \Big) +$$

$$(-1 + y) \left(- \left(\left(e^{t (-\gamma_- - \lambda_3)} \left(\frac{1}{2} \left(-\lambda_{-1} + \lambda_1 - \lambda_2 - \sqrt{\left(-4 \lambda_1 \lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) \right. \right. \right.$$

$$\left((\gamma_+ - \lambda_1)\ \lambda_1 + \frac{1}{2}\lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) +$$

$$\lambda_1 \left(\lambda_{-1}\,\lambda_1 + \frac{1}{2}\,(\gamma_+ - \lambda_1)\ \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) \Bigg) \Bigg) \Bigg/$$

$$\left((\gamma_- - \gamma_+ + \lambda_3)\ \left(\gamma_-^2 - \gamma_-\,\lambda_{-1} - \gamma_-\,\lambda_1 - \gamma_-\,\lambda_2 + \lambda_1\,\lambda_2 + 2\,\gamma_-\,\lambda_3 - \lambda_{-1}\,\lambda_3 - \lambda_1\,\lambda_3 - \lambda_2\,\lambda_3 + \lambda_3^2 \right) \right) \Bigg) -$$

$$\Bigg(e^{-t\,\gamma_+} \left(\lambda_1 \left(\lambda_{-1}\,\lambda_1 + \frac{1}{4} \left(\lambda_{-1} - \lambda_1 + \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right.\right.$$

$$\left.\left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) +$$

$$\left(\frac{1}{2}\lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) + \right.$$

$$\left. \frac{1}{2}\lambda_1 \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right)\ (\gamma_- - \lambda_{-1} - \lambda_2 + \lambda_3) \Bigg) \Bigg) \Bigg/$$

$$\left(\left(\gamma_+^2 - \gamma_+\,\lambda_{-1} - \gamma_+\,\lambda_1 - \gamma_+\,\lambda_2 + \lambda_1\,\lambda_2 \right)\ (-\gamma_- + \gamma_+ - \lambda_3) \right) + \Bigg(e^{\frac{1}{2}t \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2} \right)}$$

$$\left(\lambda_1 \left(\lambda_{-1}\,\lambda_1 + \frac{1}{2}\,(\gamma_+ - \lambda_1)\ \left(\lambda_{-1} - \lambda_1 + \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) + \right.$$

$$\left((\gamma_+ - \lambda_1)\ \lambda_1 + \frac{1}{2}\lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right)$$

$$\left. (\gamma_- - \lambda_{-1} - \lambda_2 + \lambda_3) \right) \Bigg) \Bigg/ \Bigg(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 + \gamma_-\,\lambda_1\,\lambda_2 + \gamma_+\,\lambda_1\,\lambda_2 +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 + \gamma_+\,\lambda_1\,\lambda_3 +$$

$$\gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^2$$

$$(3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 - \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)$$

$$(2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} + 2\,\gamma_-\,\lambda_1 + 2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 +$$

$$2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3) \Bigg) + \Bigg(e^{\frac{1}{2}t \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2} \right)}$$

$$\left(\lambda_1 \left(\lambda_{-1}\,\lambda_1 + \frac{1}{2}\,(\gamma_+ - \lambda_1)\ \left(\lambda_{-1} - \lambda_1 + \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right) + \right.$$

$$\left((\gamma_+ - \lambda_1)\ \lambda_1 + \frac{1}{2}\lambda_1 \left(-\lambda_{-1} + \lambda_1 - \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) \right)$$

$$\left. (\gamma_- - \lambda_{-1} - \lambda_2 + \lambda_3) \right) \Bigg) \Bigg/ \Bigg(\gamma_-\,\gamma_+\,\lambda_{-1} + \gamma_-\,\gamma_+\,\lambda_1 + \gamma_-\,\gamma_+\,\lambda_2 + \gamma_-\,\lambda_1\,\lambda_2 + \gamma_+\,\lambda_1\,\lambda_2 +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^3 + \gamma_+\,\lambda_{-1}\,\lambda_3 + \gamma_+\,\lambda_1\,\lambda_3 +$$

$$\gamma_+\,\lambda_2\,\lambda_3 + \lambda_1\,\lambda_2\,\lambda_3 + \frac{1}{4} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right)^2$$

$$(3\,\gamma_- + 3\,\gamma_+ + 3\,\lambda_{-1} + 3\,\lambda_1 + 3\,\lambda_2 + 3\,\lambda_3) +$$

$$\frac{1}{2} \left(-\lambda_{-1} - \lambda_1 - \lambda_2 + \sqrt{\left(-4\,\lambda_1\,\lambda_2 + (\lambda_{-1} + \lambda_1 + \lambda_2)^2 \right)} \right) (2\,\gamma_-\,\gamma_+ + 2\,\gamma_-\,\lambda_{-1} + 2\,\gamma_+\,\lambda_{-1} +$$

$$2\,\gamma_-\,\lambda_1 + 2\,\gamma_+\,\lambda_1 + 2\,\gamma_-\,\lambda_2 + 2\,\gamma_+\,\lambda_2 + 2\,\lambda_1\,\lambda_2 + 2\,\gamma_+\,\lambda_3 + 2\,\lambda_{-1}\,\lambda_3 + 2\,\lambda_1\,\lambda_3 + 2\,\lambda_2\,\lambda_3)\Big)\Big)\Big\}$$

Simpler examples, more details

```
In[•]:= MomentEquations[{"X" → 0}, {#}, {k}] & /@ Range[4] // Column
```

$$\mathbb{E}_X'[t] == -k\,\mathbb{E}_X[t]$$

$$\mathbb{E}_{X^2}'[t] == -k\,\mathbb{E}_X[t] - 2\,k\,(-\mathbb{E}_X[t] + \mathbb{E}_{X^2}[t])$$

$$\text{Out[•]= } \mathbb{E}_{X^3}'[t] == -k\,\mathbb{E}_X[t] - 6\,k\,(-\mathbb{E}_X[t] + \mathbb{E}_{X^2}[t]) - 3\,k\,(2\,\mathbb{E}_X[t] - 3\,\mathbb{E}_{X^2}[t] + \mathbb{E}_{X^3}[t])$$

$$\mathbb{E}_{X^4}'[t] == -k\,\mathbb{E}_X[t] - 14\,k\,(-\mathbb{E}_X[t] + \mathbb{E}_{X^2}[t]) - 18\,k\,(2\,\mathbb{E}_X[t] - 3\,\mathbb{E}_{X^2}[t] + \mathbb{E}_{X^3}[t]) - 4\,k\,(-6\,\mathbb{E}_X[t] + 11\,\mathbb{E}_{X^2}[t] - 6\,\mathbb{E}_{X^3}[t] + \mathbb{E}_{X^4}[t])$$

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In[•]:= MomentEquations[reac = {2 "Y" ← "X" + "Y" → 2 "X"}, {1, 2}, {k1, k2}]
```

$$\text{Out[•]= } \mathbb{E}_{X\,Y^2}'[t] == 3\,k_1\,(\mathbb{E}_{X^2\,Y}[t] - \mathbb{E}_{X\,Y}[t]) - k_2\,(\mathbb{E}_{X^2\,Y}[t] - \mathbb{E}_{X\,Y}[t]) - k_1\,(\mathbb{E}_{X\,Y^2}[t] - \mathbb{E}_{X\,Y}[t]) - k_2\,(\mathbb{E}_{X\,Y^2}[t] - \mathbb{E}_{X\,Y}[t]) - k_1\,\mathbb{E}_{X\,Y}[t] - k_2\,\mathbb{E}_{X\,Y}[t] + 2\,k_1\,(\mathbb{E}_{X^2\,Y^2}[t] - \mathbb{E}_{X^2\,Y}[t] - \mathbb{E}_{X\,Y^2}[t] + \mathbb{E}_{X\,Y}[t]) - 2\,k_2\,(\mathbb{E}_{X^2\,Y^2}[t] - \mathbb{E}_{X^2\,Y}[t] - \mathbb{E}_{X\,Y^2}[t] + \mathbb{E}_{X\,Y}[t]) + k_2\,(-3\,\mathbb{E}_{X\,Y^2}[t] + \mathbb{E}_{X\,Y^3}[t] + 2\,\mathbb{E}_{X\,Y}[t]) - k_1\,(-3\,\mathbb{E}_{X\,Y^2}[t] + \mathbb{E}_{X\,Y^3}[t] + 2\,(\mathbb{E}_{X\,Y^2}[t] - \mathbb{E}_{X\,Y}[t]) + 2\,\mathbb{E}_{X\,Y}[t])$$

```
In[•]:= MasterEquation[reac, {k2, k1}, {t, x, y}, P]
```

$$\text{Out[•]= } \left\{P^{(1,0,0)}[t, x, y] == (-1 + x)\,(1 + y)\,P[t, -1 + x, 1 + y]\,k_1 + (1 + x)\,(-1 + y)\,P[t, 1 + x, -1 + y]\,k_2 - P[t, x, y]\,(x\,y\,k_1 + x\,y\,k_2)\right\}$$

```
In[•]:= pgfe = ProbabilityGeneratingFunctionEquation[reac, {k2, k1}, {t, z1, z2}, G]
```

$$\text{Out[•]= } G^{(1,0,0)}[t, z_1, z_2] == k_1\left(z_1^2 - z_1\,z_2\right)G^{(0,1,1)}[t, z_1, z_2] + k_2\left(-z_1\,z_2 + z_2^2\right)G^{(0,1,1)}[t, z_1, z_2]$$

```
In[•]:= StationaryProbabilityDistributionEquation[reac, {k2, k1}, {x, y}, P]
```

$$\text{Out[•]= } \{(-1 + x)\,(1 + y)\,P[-1 + x, 1 + y]\,k_1 + (1 + x)\,(-1 + y)\,P[1 + x, -1 + y]\,k_2 - P[x, y]\,(x\,y\,k_1 + x\,y\,k_2) == 0\}$$

```
In[•]:= RSolve[
 StationaryProbabilityDistributionEquation[reac, {k2, k1}, {x, y}, P], P[x, y], {x, y}]
```

$$\text{Out[•]= } \left\{\left\{P[x, y] \to -\frac{C[1][x + y]}{x\,y} + \left(\left(1 - \left(\frac{k_1}{k_2}\right)^x\right)k_2^2\,C[2][x + y]\right)\Big/\,(x\,y\,k_1\,(k_1 - k_2))\right\}\right\}$$

```
In[•]:= dm = DeterministicModel[reac, {k2, k1}, {x, y}, t][[1]]
```

$$\text{Out[•]= } \{x'[t] == k_1\,x[t]\,y[t] - k_2\,x[t]\,y[t],\ y'[t] == -k_1\,x[t]\,y[t] + k_2\,x[t]\,y[t]\}$$

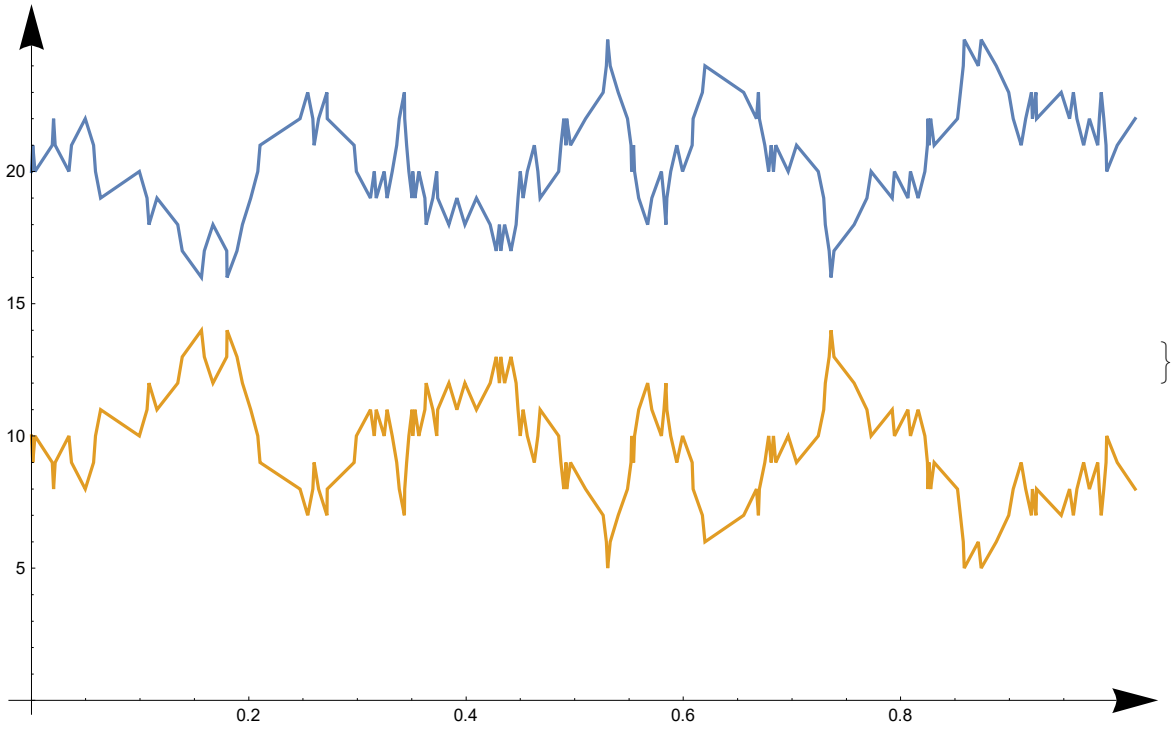
```
In[•]:= dm[[1]] /. {y[t] → x0 + y0 - x[t]} // Simplify
```

$$\text{Out[•]= } x'[t] == (k_1 - k_2)\,(x_0 + y_0 - x[t])\,x[t]$$

Simulation

```
SeedRandom[500];
sp1 = SimulationPlot[{"X" ⇌ "Y"}, {3.8, 8.3},
    {20, 10}, 1, Verbose → True, ImageSize → 600] // Timing
```

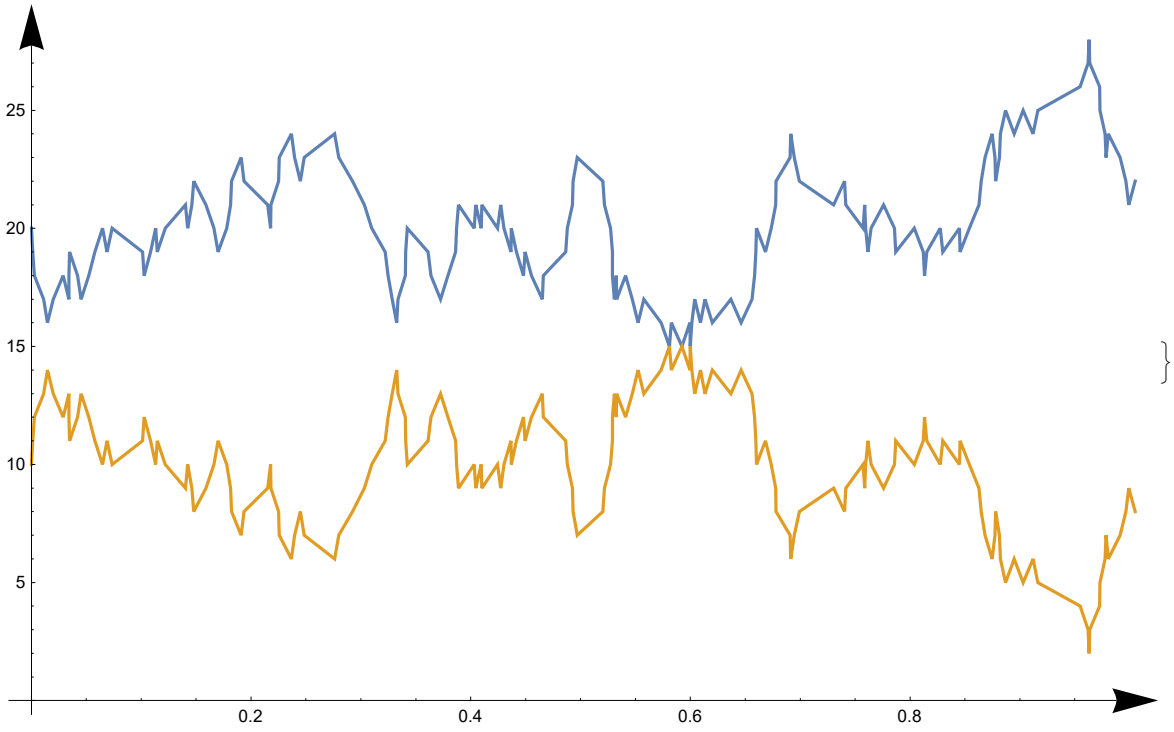
```
{0.140625,
```




```
}
```

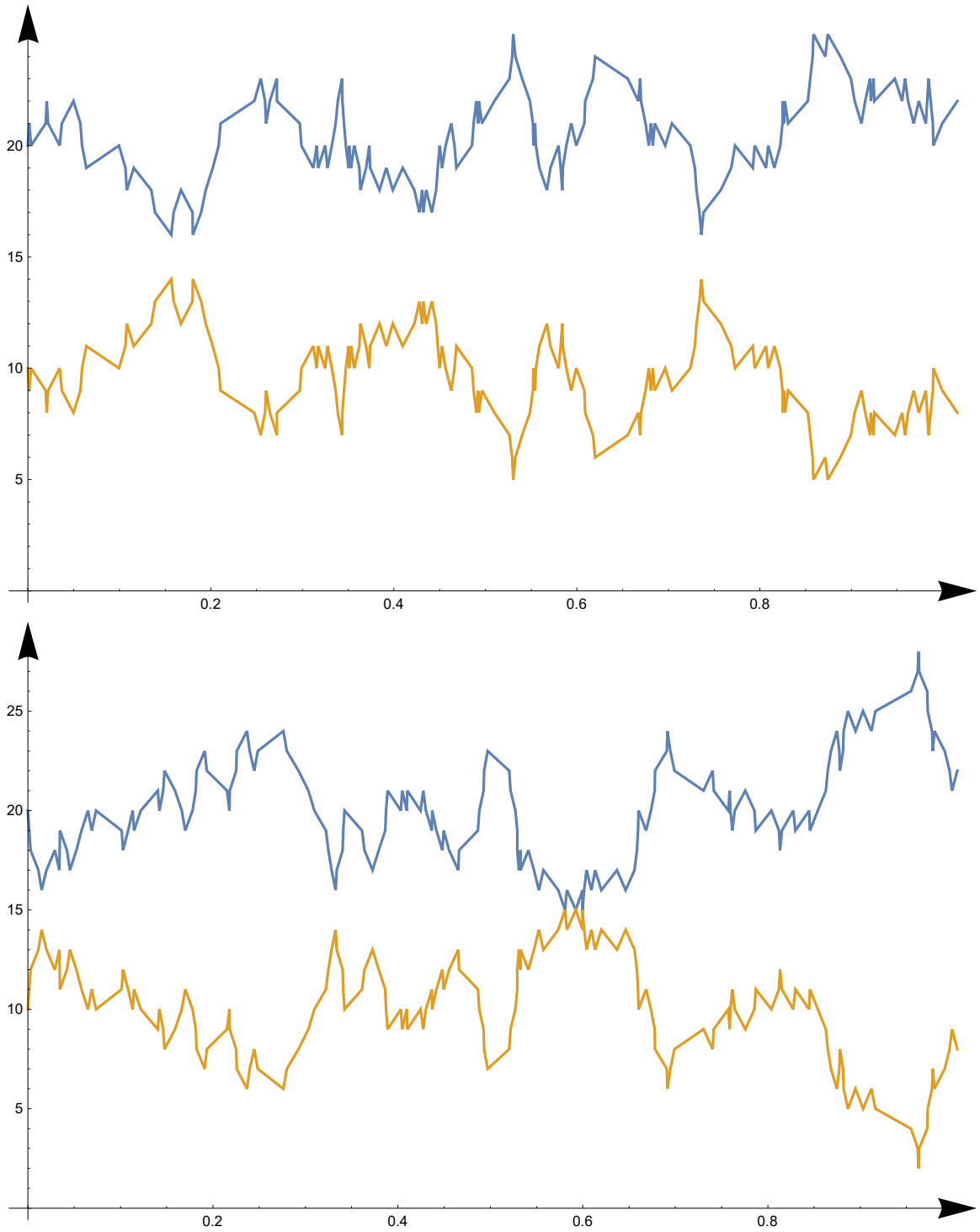
```
SeedRandom[1];
sp2 = SimulationPlot[{"X" ⇌ "Y"}, {3.8, 8.3},
    {20, 10}, 1, Verbose → True, ImageSize → 600] // Timing
```

```
{0.09375,
```

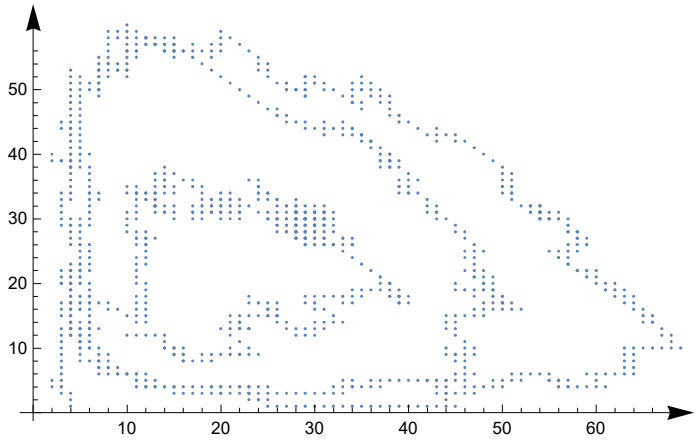



```
}
```

```
differentsimul = Column[Last /@ {sp1, sp2}]
```



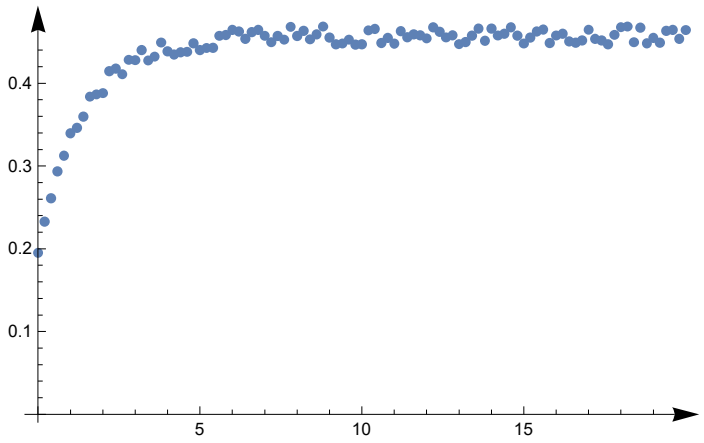
```
SeedRandom[1];
SimulationPlot2D[{"Lotka-Volterra"},
 {2, 0.1, 2}, {10, 12}, 10, ExternalSpecies → {"A", "B"}]
```



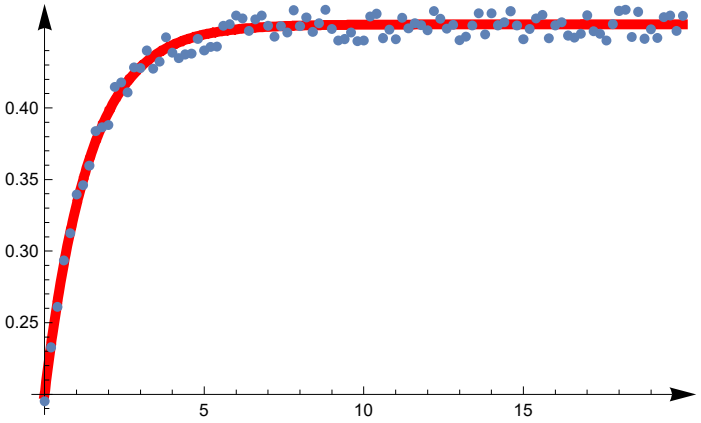
Inverse problems

Parameter estimation

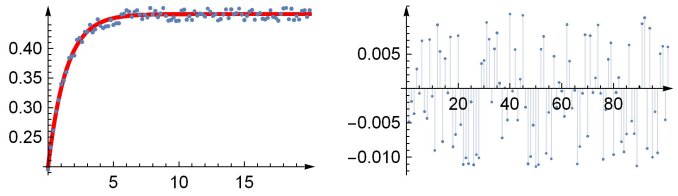
```
ClearAll[sol, times, data];
sol := First[ReplaceAll @@ Concentrations[{0 ⇔ "X"}, {0.33, 0.72}, {0.2}, {0, 20}]]
times = N[Range[0, 100] / 5]; SeedRandom[100];
data = Transpose[{times, (sol /. t → times) (1 + RandomReal[{-0.025, 0.025}, 101])}];
simdata = ListPlot[data, PlotRange → All, PlotStyle → Directive[PointSize[0.015]]]
```



```
ClearAll[a, b, model2, nlm2, pl2];
model2[a_?NumberQ, b_?NumberQ, c_?NumberQ] :=
  (model[a, b, c] = Function[t, Evaluate[First[
       ReplaceAll @@ Concentrations[{0 ⇔ "X"}, {0.33, 0.72}, {0.2}, {0, 20}]]]]);
nlm2 = NonlinearModelFit[data, model2[a, b, c][t], {{a, .1}, {b, .1}, {c, 1}}, t]; //
 Quiet
pl2 = Plot[Evaluate[nlm2[t]], {t, 0, 20}, PlotRange → All,
  PlotStyle → Directive[Red, Thickness[0.015]], Epilog → First@simdata,
  ImagePadding → {{Automatic, Automatic}, {10, 10}}]
```




```
lp2 = ListPlot[nlm2["FitResiduals"], Filling → Axis,
    ImagePadding → {{Automatic, Automatic}, {10, 10}}];
GraphicsRow[{pl2, lp2}]
```




```
nlm2["Properties"]
```

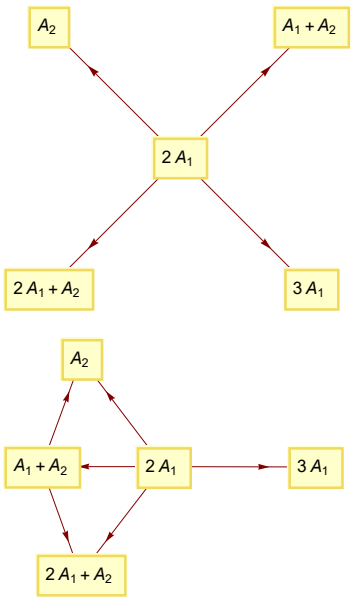
```
{AdjustedRSquared, AIC, AICc, ANOVATable, ANOVATableDegreesOfFreedom,
 ANOVATableEntries, ANOVATableMeanSquares, ANOVATableSumsOfSquares,
 BestFit, BestFitParameters, BIC, CorrelationMatrix, CovarianceMatrix,
 CurvatureConfidenceRegion, Data, EstimatedVariance, FitCurvatureTable,
 FitCurvatureTableEntries, FitResiduals, Function, HatDiagonal, MaxIntrinsicCurvature,
 MaxParameterEffectsCurvature, MeanPredictionBands, MeanPredictionConfidenceIntervals,
 MeanPredictionConfidenceIntervalTable, MeanPredictionConfidenceIntervalTableEntries,
 MeanPredictionErrors, ParameterBias, ParameterConfidenceIntervals,
 ParameterConfidenceIntervalTable, ParameterConfidenceIntervalTableEntries,
 ParameterConfidenceRegion, ParameterErrors, ParameterPValues, ParameterTable,
 ParameterTableEntries, ParameterTStatistics, PredictedResponse, Properties,
 Response, RSquared, SingleDeletionVariances, SinglePredictionBands,
 SinglePredictionConfidenceIntervals, SinglePredictionConfidenceIntervalTable,
 SinglePredictionConfidenceIntervalTableEntries,
 SinglePredictionErrors, StandardizedResiduals, StudentizedResiduals}
```

Finding reaction to a given (kinetic) differential equation

Reactions with the same deterministic model

Different structures

```
Column[ShowFHJGraph[#] & /@ {{2 A1 → A2, 2 A1 → 2 A1 + A2, 2 A1 → 3 A1, 2 A1 → A1 + A2},
    {2 A1 → A2, 2 A1 → 2 A1 + A2, 2 A1 → 3 A1, 2 A1 → A1 + A2, A1 + A2 → 2 A1 + A2, A1 + A2 → A2}}]
```

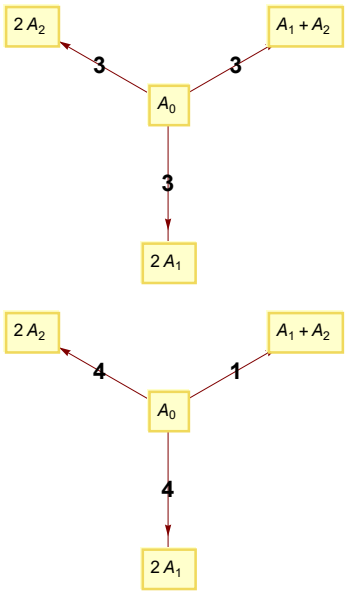



```
MapThread[RightHandSide[#1, #2, {x, y}] &,
 {{{2 A1 → A2, 2 A1 → 2 A1 + A2, 2 A1 → 3 A1, 2 A1 → A1 + A2},
   {2 A1 → A2, 2 A1 → 2 A1 + A2, 2 A1 → 3 A1, 2 A1 → A1 + A2, A1 + A2 → 2 A1 + A2, A1 + A2 → A2}},
  {Array[1 &, 4], {1, 19 / 10, 1 / 10,
    1 / 10, 1 / 10, 1 / 10}}}]
```

$$\left\{\left\{-2\,x^2,\ 3\,x^2\right\},\ \left\{-2\,x^2,\ 3\,x^2\right\}\right\}$$

Different reaction rate coefficients

```
Column[{ShowFHJGraph[craciunpantea = {"A0" → 2 "A2", "A0" → 2 "A1", "A0" → "A1" + "A2"},
    Style[#, Bold, 12] & /@ {3, 3, 3}],
  ShowFHJGraph[craciunpantea, Style[#, Bold, 12] & /@ {4, 4, 1}]}]
```




```
RightHandSide[{craciunpantea}, #] & /@ {{3, 3, 3}, {4, 4, 1}}
```

$$\{\{-9\, c_{A_0},\ 9\, c_{A_0},\ 9\, c_{A_0}\},\ \{-9\, c_{A_0},\ 9\, c_{A_0},\ 9\, c_{A_0}\}\}$$

Reaction with no effect on the rhs

```
DeterministicModel[{2 "Y" ← "X" + "Y" → 2 "X"}, {k, k}, {x, y}][[1]]
```

$$\{x'[t] == 0,\ y'[t] == 0\}$$

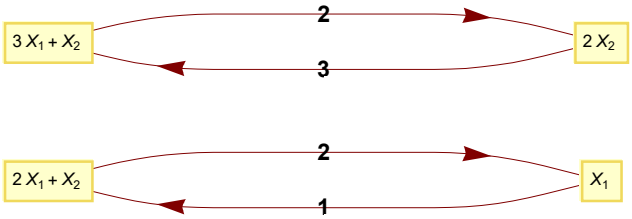
Inducing reactions with best properties (zero deficiency, weak reversibility etc.)

If you want to find them, start here:

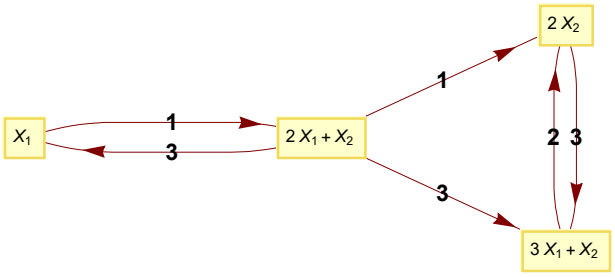
```
Hyperlink["Szederkényi",
 "https://scholar.google.hu/citations?user=-f46rMcAAAAJ&hl=hu&oi=ao"]
```

Szederkényi

```
dyneqsteps1 = {"X1" ⇌ 2 "X1" + "X2", 2 "X2" ⇌ 3 "X1" + "X2"};
dyneq1 = ShowFHJGraph[dyneqsteps1, Style[#, Bold, 12] & /@ {1, 2, 3, 2}]
```




```
dyneqsteps2 = {"X1" ⇌ 2 "X1" + "X2" → 2 "X2" ⇌ 3 "X1" + "X2" ← 2 "X1" + "X2"};
dyneq2 = ShowFHJGraph[dyneqsteps2, Style[#, Bold, 12] & /@ {1, 3, 1, 3, 2, 3}]
```




```
szeder1 = {2 A1 → A2, 2 A1 → A1 + A2, 2 A1 → 3 A1, 2 A1 → 2 A1 + A2};

s1 = ShowFHJGraph[szeder1, Array[1 &, 4], DirectedEdges -> True, VertexLabeling → True]

figurexp["TothNagyPapp-Fig11.5A", s1]

szeder2 =
  {2 A1 → A2, 2 A1 → A1 + A2, 2 A1 → 3 A1, 2 A1 → 2 A1 + A2, A1 + A2 → A2, A1 + A2 → 2 A1 + A2};

s2 = ShowFHJGraph[szeder2, {1, 0.1, 0.1, 1.9, 0.1, 0.1},
  DirectedEdges -> True, VertexLabeling → True]

origr = {X + Y ⇔ X + 2 Y ⇔ 2 X + 3 Y → 2 Y ← X + Y, 2 Y ⇔ X + 2 Y};

orig = ShowFHJGraph[origr,
  Style[#, Bold, 16] & /@ ({"k1", "k2", "k5", "k4", "k8", "k3", "k7", "k6"} /.
     {"k1" → 1, "k2" → "11/10", "k5" → "11/10", "k4" → 1, "k8" → 1,
      "k3" → 1 , "k7" → 3, "k6" → "1/10"}), ImageSize → 1300]

sparser = {X + Y ⇔ X + 2 Y ⇔ 2 X + 3 Y → 2 Y ← X + Y, 2 Y → X + 2 Y};

sparse = ShowFHJGraph[sparser,
  Style[#, Bold, 16] & /@ ({"k1", "k2", "k3", "k4", "k5", "k6", "k7"} /. {"k1" → 1,
       "k2" → 1, "k3" → 1, "k4" → 1, "k5" → 1, "k6" → 1, "k7" → 3}), ImageSize → 1000]

denser = {2 X + 3 Y ⇔ X + Y ⇔ X + 2 Y ⇔ 2 X + 3 Y ⇔ 2 Y ⇔ X + Y, 2 Y ⇔ X + 2 Y};

dense = ShowFHJGraph[denser, Style[#, Bold, 16] & /@
    ({"k1", "k2", "k3", "k4", "k5", "k6", "k7", "k8", "k9", "k10", "k11", "k12"} /.
      {"k1" → "3/10", "k2" → "3/10", "k3" → "1/10", "k4" → "11/10" , "k5" → "11/10",
       "k6" → "1/10", "k7" → "13/10", "k8" → "29/30" , "k9" → "29/30" ,
       "k10" → "13/10" , "k11" → "1/10", "k12" → "1/10"}), ImageSize → 800]
```

Identifiablility and Uniqueness Questions

No compartmental system induces this kinetic differential equation

```
RightHandSide[{"Y" → 3 "X", "X" → 3 "Y"}, {1, 1}, {x, y}]
```

```
{-x + 3 y, 3 x - y}
```

Programs

Other programs

```
Hyperlink["Demonstrations", "http://demonstrations.wolfram.com/"]
```

Ferreira MMC, Ferreira WCJ, Lino ACS, Porto MEG: Uncovering oscillations, complexity, and chaos in chemical kinetics using Mathematica. *J Chem Educ* **76**(6) (1999), 861–866.

Francl MM (2000) Introduction to the use of numerical methods in chemical kinetics.

```
Hyperlink["Francl", "http://ckw.phys.ncku.edu.tw/public/pub/WebSources/MathSource/
library.wolfram.com/infocenter/MathSource/791/index.html"]
```

```
Francl
```

Hollis S (2004) Reaction-diffusionlab.m.

```
Hyperlink["Hollis", "http://www.math.armstrong.edu/faculty/hollis/mmade/RDL"]
```

Kyurkchiev N, Markov S, Mincheva M.: Analysis of biochemical mechanisms using Mathematica with applications. Serdica J. Computing 10 (2016), No 1, 63–78

Mulquiney PM, Kuchel PW (2003) Modelling metabolism with Mathematica. CRC Press, Boca Raton, FL, URL

```
Hyperlink["Kuchel, includes CD-ROM",
 "http://www.bioeng.auckland.ac.nz/MCF/invited_users/philip_kuchel.htm"]
```

Sánchez G (2005) Biokmod: A Mathematica toolbox for modeling biokinetic systems. Mathematica in Education and Research 10(2):1–34, URL

```
Hyperlink["Sanchez", "http://diarium.usal.es/guillermo/biokmod/"]
```

Information about our ReactionKinetics.wl

```
Hyperlink["Springer", "http://extras.springer.com"]
```

```
Springer
```

In[8]:=
```
OpenReactionKineticsPalette[]
```

Out[8]=
```
NotebookObject[ ReactionKinetics Palette ]
```

In[9]:=
```
Names["ReactionKinetics`*"]
```

Out[9]=
```
{AbsoluteConcentrationRobustness, AcyclicVolpertGraphQ, AtomConservingQ, Atoms,
 AtomsQ, AvogadrosNumber, BioModels, BioReactions, Bipartite, CHEMKINExport,
 CHEMKINImport, CombinatorialMoments, ComplexColors, ComponentwiseLessEqualQ,
 Concentrations, Conditions, ContejeanDevie, CoveringDecompositionSet,
 Decompositions, DeleteAutocatalysis, DependencyGraph, DetailedBalanced,
 DeterministicModel, EdgeLabeled, EigensystemJacobian, ElementaryReactions,
 ExternalSpecies, FastSelection, Filter, FilterReactions, FixedStepSize,
 FormattedOutput, FromAtomMatrix, FromStoichiometry, GammaLeftNullSpace,
 GeneratedRateCoefficient, GetReaction, GreedySelection, Highlight, LPBased,
 MassAction, MassActionKinetics, MassConservationRelations, MasterEquation,
 MaxFHJStronglyConnectedComponents, MaxFHJWeaklyConnectedComponents, MaxIteration,
 Memo, MinFHJStronglyConnectedComponents, MinFHJWeaklyConnectedComponents,
 MinimalDecompositions, Models, MolarGasConstant, MomentEquations, Numbered,
 ObjectiveFunction, Obligatory, Omittable, OpenReactionKineticsNamesPalette,
 OpenReactionKineticsPalette, OriginalSelection, PlotFunction, Positivity,
 Preprocess, ProbabilityGeneratingFunctionEquation, ReactionRatesNotebook,
 Reactions, ReactionsData, ReversibleFHJRepresentation, ReversibleQ, RightHandSide,
 SelectMinimalDecompositions, ShowDependencyGraph, ShowFHJGraph, ShowVolpertGraph,
 Side, Simulation, SimulationPlot, SimulationPlot2D, SimulationPlot3D,
 SolveProbabilityGeneratingFunctionEquation, Species, StationaryPoints,
 StationaryProbabilityDistributionEquation, StronglyConnectedComponentsColors,
 SubgraphHighlight, TimeLimit, ToAtomMatrix, ToCanonicalForm, ToReversible,
 VolpertIndexing, WeaklyReversibleQ, ZeroVectorQ, $ReactionKinetics,
 $ReactionKineticsPackageLoaded, $ReactionKineticsVersionNumber}
```

In[10]:=
```
Information["ReactionKinetics`*"]
```

▼ ReactionKinetics`

AbsoluteConcentrationRobustness
AcyclicVolpertGraphQ
AtomConservingQ
Atoms
AtomsQ
AvogadrosNumber
BioModels
BioReactions
Bipartite
CHEMKINExport
CHEMKINImport
CombinatorialMoments
ComplexColors
ComponentwiseLessEqualQ
Concentrations
Conditions
ContejeanDevie
CoveringDecompositionSet

Decompositions
DeleteAutocatalysis
DependencyGraph
DetailedBalanced
DeterministicModel
EdgeLabeled
EigensystemJacobian
ElementaryReactions
ExternalSpecies
FastSelection
Filter
FilterReactions
FixedStepSize
FormattedOutput
FromAtomMatrix
FromStoichiometry
GammaLeftNullSpace
GeneratedRateCoefficient
GetReaction
GreedySelection
Highlight
LPBased
MassAction
MassActionKinetics
MassConservationRelations
MasterEquation
MaxFHJStronglyConnectedComponents
MaxFHJWeaklyConnectedComponents
MaxIteration
Memo
MinFHJStronglyConnectedComponents
MinFHJWeaklyConnectedComponents
MinimalDecompositions
Models
MolarGasConstant
MomentEquations
Numbered
ObjectiveFunction
Obligatory
Omittable
OpenReactionKineticsNamesPalette
OpenReactionKineticsPalette

OriginalSelection
PlotFunction
Positivity
Preprocess
ProbabilityGeneratingFunctionEquation
ReactionRatesNotebook
Reactions
ReactionsData
ReversibleFHJRepresentation
ReversibleQ
RightHandSide
SelectMinimalDecompositions
ShowDependencyGraph
ShowFHJGraph
ShowVolpertGraph
Side
Simulation
SimulationPlot
SimulationPlot2D
SimulationPlot3D
SolveProbabilityGeneratingFunctionEquation
Species
StationaryPoints
StationaryProbabilityDistributionEquation
StronglyConnectedComponentsColors
SubgraphHighlight
TimeLimit
ToAtomMatrix
ToCanonicalForm
ToReversible
VolpertIndexing
WeaklyReversibleQ
ZeroVectorQ
$ReactionKinetics
$ReactionKineticsPackageLoaded
$ReactionKineticsVersionNumber

AbsoluteConcentrationRobustness[{reactions},options]
checks the Shinar–Feinberg conditions for the reaction.

```
Attributes[AbsoluteConcentrationRobustness] = {Protected, ReadProtected}
```

```
Options[AbsoluteConcentrationRobustness] := {TimeLimit → 120, ExternalSpecies → {}}
```

In[11]:= **? Concentrations**

Concentrations[{reactions},rates,initvalues,vars,options] attempts to solve the induced kinetic differential equation endowed with some kinetics described by the rates. Initial concentrations are given by initvalues, vars contain the names of the independent variables. This way Concentrations uses DSolve, accepts symbolic parameters, and tries to return the symbolic solution to the equation (i.e. concentrations versus time curves).

Concentrations[{reactions},rates,initvalues,{t0,t1},vars,options] uses NDSolve to give the numerical solution from t0 to t1.

Concentrations[{reactions},arrheniuscoeffs,enthalpies,c0,V,Ta,tres,p1,p2,initvalues,{t0,t1},options] tries to solve the general evolution equation for reactions involving temperature effects. In this case the kinetics is assumed to be of the mass action type, the temperature dependence is allowed to be of the generalized Arrhenius type. The Arrhenius triples are given by arrheniuscoeffs.

In[12]:= **? Simulation**

Simulation[{reactions},rratecoeffs,init,maxtime,options] simulates the induced kinetic Markov process of the reaction endowed with stochastic mass action type kinetics with stochastic reaction rate coefficients given by rratecoeffs. The initial state are given by init, while the stopping time is specified by maxtime.

Options include ExternalSpecies, FixedStepSize, Tolerance (for tau–leaping), MaxIteration, Method, Verbose and Volume.

The following methods can be used: "Direct" (default), "FirstReaction", "NextReaction", "ExplicitTau–Leaping", "ImplicitTau–Leaping" and "TrapezoidalTau–Leaping".

? SimulationPlot

SimulationPlot[{reactions},rratecoeffs,init,maxtime,options] simulates and plots the trajectories of species, where the induced kinetic Markov endowed with stochastic mass action type kinetics with stochastic reaction rate coefficients given by rratecoeffs.

Options include ExternalSpecies, PlotFunction (default is "ListLinePlot") and Species (default is All).

In[13]:= **Options[ShowFHJGraph]**

Out[13]= {ExternalSpecies → {}, ComplexColors → {}, PlotFunction → GraphPlot, StronglyConnectedComponentsColors → {}, Numbered → False}

? ShowFHJGraph

In[14]:= **Models**

Out[14]= {Autocatalator, Belousov-Zhabotinsky, Briggs-Rauscher, Brusselator, Chapman cycle, Clarke, Colquhoun, Consecutive, Decomposition, DeYoung-Keizer, Dimerization, Edelstein, Eigen, Érdi-Ropolyi, Explodator, Horn-Jackson, Feinberg-Horn I, Feinberg-Horn II, FKN mechanism, Frank, Goldbeter, Hudson-Rössler, Huxel, Hyver, Inflow, Ivanova, Kliemann, Leonard-Reichl, Lotka, Lotka-Volterra, Michaelis-Menten, Mole, Ogg, Oregonator, Outflow, Petri, Robertson, Schlögl, Simple birth-death, Triangle, Turányi-Györgyi-Field, Vaiman, Verhulst, Volpert, Wegscheider, Willamowski-Rössler}

In[15]:= **BioModels**

Out[15]= {Calvin Cycle (Photosynthesis), Glycolysis, Glyoxylate Cycle, SzentGyörgyi–Krebs Cycle}

In[16]:= **Reactions**

Out[16]=
$$\Big\{\text{Autocatalator} \to \{A \to X,\ X \to Y,\ X + 2\,Y \to 3\,Y,\ Y \to P\},$$

$$\text{Belousov–Zhabotinsky} \to \Big\{H + X + Y \to 2\,V,\ A + 2\,H + Y \to V + X,\ 2\,X \to V,$$

$$A + H + \frac{X}{2} \to X + Z,\ X + Z \to \frac{X}{2},\ M + Z \to Q,\ V + Z \to Y,\ V \to Y,\ X \to 0,\ Y \to 0,\ Z \to 0,\ V \to 0\Big\},$$

$$\text{Briggs–Rauscher} \to \{CH2(CO2H)2 + H^{+} + 2\,H2O2 + IO3^{-} \to 3\,H2O + ICH(CO2H)2 + 2\,O2,$$

$$H^{+} + 2\,H2O2 + IO3^{-} \to 2\,H2O + HIO + 2\,O2,\ CH2(CO2H)2 + HIO \to H2O + ICH(CO2H)2,$$

$$2\,H^{+} + I^{-} + IO3^{-} \to HIO + HIO2,\ H^{+} + HIO2 + I^{-} \to 2\,HIO,$$

$$H2O2 + HIO \to H^{+} + H2O + I^{-} + O2,\ H^{+} + HIO2 + IO3^{-} \to H2O + 2\,IO2,$$

$$H2O + IO2 + Mn^{2+} \to HIO2 + Mn(OH)^{2+},\ H2O2 + Mn^{2+} \to H2O + HO2 + Mn^{2+},$$

$$2\,HO2 \to H2O2 + O2,\ 2\,HIO2 \to H^{+} + HIO + IO3^{-},$$

$$H^{+} + HIO + I^{-} \to H2O + I2,\ CH2(CO2H)2 + I2 \to H^{+} + I^{-} + ICH(CO2H)2\},$$

$$\text{Brusselator} \to \{X \leftarrow A,\ B + X \to D + Y,\ 2\,X + Y \to 3\,X,\ X \to E\},$$

$$\text{Chapman cycle} \to \{O2 \to 2\,O,\ M + O + O2 \to M + O3,\ O3 \to O + O2,\ O + O3 \to 2\,O2\},$$

$$\text{Clarke} \to \{A + T \to M + S,\ H + T + Y \to S + V,\ H + X + Y \to 2\,T,\ B + 2\,H + Y \to T + X,\ 2\,X \to B + H + T,$$

$$B + H + X \to S + 2\,U,\ H + U + W \to X + Z,\ S + U + Z \to B + 2\,H + W,\ A + V \to H + M + Y,$$

$$A + 2\,S + 6\,Z \to 6\,H + P + 2\,Q + 6\,W,\ M + 2\,S + 4\,Z \to 5\,H + P + 2\,Q + 4\,W + Y,\ P + T \to H + Q + S + Y\},$$

$$\text{Colquhoun} \to \{AR \rightleftharpoons A + R \rightleftharpoons RA,\ A + AR \rightleftharpoons ARA \rightleftharpoons A + RA\},\ \text{Consecutive} \to \{A \to B \to C\},$$

$$\text{Decomposition} \to \{C \to A + B\},$$

$$\text{DeYoung–Keizer} \to \{S(000) \rightleftharpoons S(001) \rightleftharpoons S(100) \rightleftharpoons S(010),$$

$$S(100) \rightleftharpoons S(101) \rightleftharpoons S(110),\ S(001) \rightleftharpoons S(101) \rightleftharpoons S(011),$$

$$S(011) \rightleftharpoons S(010) \rightleftharpoons S(111),\ S(110) \rightleftharpoons S(010) \rightleftharpoons S(111),\ S(111) \rightleftharpoons S(101)\},$$

$$\text{Dimerization} \to \{A + B \to C\},\ \text{Edelstein} \to \{X \Leftrightarrow 2\,X,\ X + Y \Leftrightarrow Z \Leftrightarrow Y\},$$

$$\text{Eigen} \to \{X \to 0,\ X \to 2\,X\},\ \text{Érdi–Ropolyi} \to \{R + 4\,T \rightleftharpoons T4R1 \rightleftharpoons T4R2 \rightleftharpoons T4R3\},$$

$$\text{Explodator} \to \{A + X \to X\,(1 + \text{aExplodator}),\ X + Y \to Z,\ Z \to Y\,(1 + \text{bExplodator}),\ Y \to P\},$$

$$\text{Horn–Jackson} \to \{3\,X \to X + 2\,Y \to 3\,Y \to 2\,X + Y \to 3\,X\},$$

$$\text{Feinberg–Horn I} \to \{2\,J \to G,\ 2\,J \leftrightarrow H,\ G \to H,\ A + B \to G,\ A + B \leftrightarrow C,\ C \to D + E,\ D + E \leftrightarrow F\},$$

$$\text{Feinberg–Horn II} \to \{X \to Y,\ X + Z \to T \to U + Y \to X + Z\},\ \text{FKN mechanism} \to$$

$$\{Br^{-} + HBrO2 \to 2\,HOBr,\ Br^{-} + BrO3^{-} \to HBrO2 + HOBr,\ 2\,HBrO2 \to BrO3^{-} + HOBr,$$

$$Br^{-} + HOBr \to Br2 + H2O,\ BrO3^{-} + HBrO2 \to 2\,BrO2 + H2O,\ H2O + HBrO2 \to BrO3^{-},$$

$$Br2 + MA \to Br^{-} + BrMA,\ 2\,H2O + MA \to 2\,CO2 + C,\ BrMA + 2\,H2O \to Br^{-} + 2\,CO2 + HCO2H\},$$

$$\text{Frank} \to \{A \to R,\ A \to S,\ A + R \to 2\,R,\ A + S \to 2\,S\},\ \text{Goldbeter} \to \{M \rightleftharpoons 0 \rightleftharpoons C,\ 0 \rightleftharpoons X,\ C \to 0\},$$

$$\text{Hudson–Rössler} \to \{P \to A,\ Q \to B,\ A + B \to 2\,B,\ B \to R,\ A \leftrightarrow C\},$$

$$\text{Huxel} \to \{X \rightleftharpoons 2\,X,\ X + Y \to 2\,Y,\ Y \to 0\},\ \text{Hyver} \to \{K1 \to A1 \to A2 \to A3 \to A4 \to A5 \to A6 \to A7,$$

$$A7 + B \to C + E,\ K \to B \to 0,\ A1 + E \to 0,\ A1 + C \to 0,\ \mu \to D,\ C + D \to 0,\ D + E \to 0\},$$

$$\text{Inflow} \to \{0 \to X\},\ \text{Ivanova} \to \{X + Y \to 2\,Y,\ Y + Z \to 2\,Z,\ X + Z \to 2\,X\},$$

$$\text{Kliemann} \to \{X \rightleftharpoons Y,\ 2\,X \rightleftharpoons X + Y \rightleftharpoons 2\,Y\},\ \text{Leonard–Reichl} \to \{2\,X \leftrightarrows Y\},$$

$$\text{Lotka} \to \{A \to X,\ X + Y \to 2\,Y,\ Y \to P\},\ \text{Lotka–Volterra} \to \{A + X \to 2\,X,\ X + Y \to 2\,Y,\ B \leftarrow Y\},$$

$$\text{Michaelis–Menten} \to \{E + S \rightleftharpoons C \to E + P\},\ \text{Mole} \to \{X + Y \to 2\,X + 2\,Y,\ X \leftrightarrow 0 \leftrightarrow Y\},$$

$$\text{Ogg} \to \{N_2O_5 \leftrightarrow NO_2 + NO_3,\ NO_2 + NO_3 \to NO + NO_2 + O_2,\ NO + NO_3 \to 2\,NO_2\},$$

$$\text{Oregonator} \to \{A + Y \to X,\ X + Y \to P,\ B + X \to 2\,X + Z,\ 2\,X \to Q,\ Z \to Y\,\text{fOregonator}\},$$

$$\text{Outflow} \to \{X \to 0\},\ \text{Petri} \to \{C + O_2 \to CO_2,\ NaOH + CO_2 \to NaHCO_3,\ HCl + NaHCO_3 \to NaCl + CO_2 + H_2O\},$$

$$\text{Robertson} \to \{A \to B,\ 2\,B \to B + C,\ B + C \to A + C\},$$

$$\text{Schlögl} \to \{0 \rightleftharpoons X,\ 2\,X \rightleftharpoons 3\,X\},\ \text{Simple birth–death} \to \{X \to 2\,X,\ X \to A\},$$

$$\text{Triangle} \to \{A \to B \to C \to A\},\ \text{Turányi–Györgyi–Field} \to$$

$$\{X + Y \to 2\,P,\ A + Y \to P + X,\ 2\,X \to A + P,\ A + X \to 2\,X + 2\,Z,\ X + Z \to A + 0.5\,X,\ M + Z \to Y - Z\},$$

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Vaiman → {2 K + O2 → 2 KO, H2S + K → KH2S, 2 KH2S + O2 → 2 H2O + K + KS2,
   H2S + KO → H2O + KS, KH2S + KO → H2O + K + KS, 2 KS → K + KS2, KS2 → K + S2},
Verhulst → {X ⇌ 2 X}, Volpert → {X + Y → T, Y + Z → U}, Wegscheider → {A ⇌ B, 2 A ⇌ A + B},
Willamowski-Rössler → {A + X ⇋ 2 X, X + Y ⇋ 2 Y, Q + Y ⇋ B, X + Z ⇋ C, P + Z ⇋ 2 Z}}
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Mathematical Chemistry BMETE92MM09, 4 hours/week, 5 credits; 2018/19. II. Students from ELTE are also welcome.