1 Example: autocatalysis kinetics

We consider the kinetics of an autocatalytic reaction [1]. The structure of the reactions is

$$A \xrightarrow{k_1} B$$
$$B + B \xrightarrow{k_2} C + B$$
$$B + C \xrightarrow{k_3} C + A,$$

where k_1, k_2, k_3 are the rate constants and A, B and C are the chemical species involved. The corresponding ODEs are

$$\begin{aligned} x_1' &= -k_1 x_1 + k_3 x_2 x_3 \\ x_2' &= k_1 x_1 - k_2 y_2^2 - k_3 x_2 x_3 \\ x_3' &= k_2 y_2^2 \end{aligned}$$

Given $k_1 = 0.04, k_2 = 1.0e4, k_3 = 3.0e7$, we seek the initial condition for $x_1(t = 0)$, combined with initial condition $x_2(t = 0) = 0.0$ and $x_3(t = 0) = 0.0$.

References

[1] H. H. Robertson. *Numerical analysis, an introduction, chapitre The solution of a set of reaction rate equations.* Academic Press, 1966.