A multi-parameter singular perturbation analysis of the Robertson model

Abstract.

The Robertson model describes a chemical reaction consisting of three reactants X, Y, Z, which interact according to the reaction scheme

$$X \xrightarrow{k_1} Y, \qquad Y + Y \xrightarrow{k_2} Y + Z, \qquad Y + Z \xrightarrow{k_3} X + Z.$$

With mass-action kinetics this leads to a system of three nonlinear ODEs depending on three reaction rates which act as parameters. The classical choice of the reaction rates is $k_1 = 4 \cdot 10^{-2}$, $k_2 = 3 \cdot 10^7$, $k_3 = 10^4$. Due to the very different orders of magnitudes of the three reaction rates, the dynamics of the system occurs on several widely separated timescales. As a consequence of this inherent stiffness, the Robertson model has been frequently used as a numerical test problem. However, no analytical results seem to exist.

In this talk we will provide a full asymptotic analysis of the Robertson model in the parameter regime $k_1, k_3 \ll k_2$. Our results are in excellent qualitative and quantitative agreement with the numerics. We reformulate the model as a two-parameter singular perturbation problem and combine blow-ups in parameter- and variable space, which allows to use geometric singular perturbation theory (GSPT) in this multi-parameter setting. This approach is a first step to adapt GSPT to problems depending singularly on several independent parameters.