Robertson Model

A MULTI-PARAMETER SINGULAR PERTURBATION PROBLEM

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I. Model

- The classical **Robertson model** [6] is given by

$$\begin{aligned}\dot{x} &= -k_1 x + k_3 yz\\ \dot{y} &= k_1 x - k_2 y^2 - k_3 yz\\ \dot{z} &= k_2 y^2,\end{aligned} \qquad (1)$$

with $k_1 = 4 \cdot 10^{-2}$, $k_2 = 3 \cdot 10^7$, $k_3 = 10^4$ and initial value $(x, y, z)^T = (1, 0, 0)^T$, where $x, y, z \geq 0$ is of interest.

- The ODE (1) is a famous stiff test problem for numerical solvers, e.g. explicit Runge-Kutta method (Figure 1) vs. implicit stiff solver BDF (Figure 2):

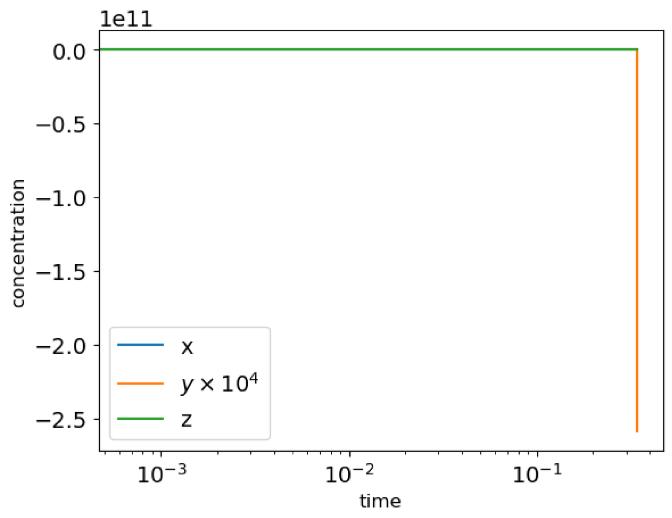

Figure 1: Numerics with RK45.

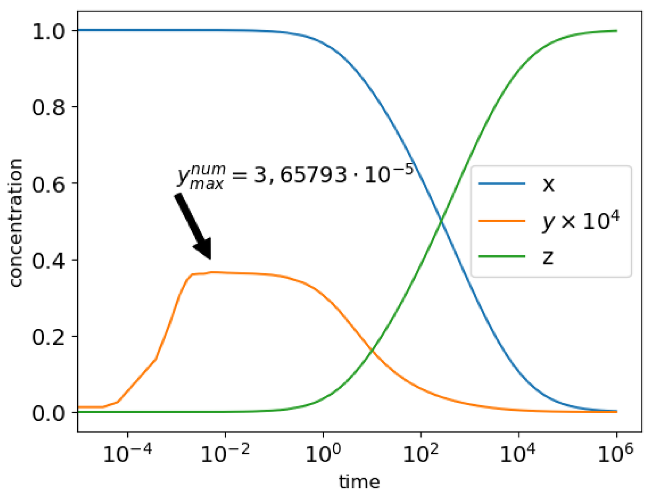

Figure 2: Numerics with BDF. Note the logarithmic time scale.

- Goal: Asymptotic analysis by Geometric Singular Perturbation Theory (GSPT), e.g. [2, 5].

II. Scalings and Singular Limits

- Assumption: Second reaction is the fastest, i.e., $k_2 >> k_1, k_3$.
- Conservation of mass $\dot{x} + \dot{y} + \dot{z} = 0$, change to the fast time $\tau = k_2 t$, define $\frac{k_1}{k_2} =: \tilde{k}_1$, $\frac{k_3}{k_2} =: \tilde{k}_3$. Dropping the $\tilde{(\cdot)}$

$$\begin{aligned}y' &= k_1(c - y - z) - y^2 - k_3 yz\\ z' &= y^2,\end{aligned} \qquad (2)$$

where $(\cdot)'$ denotes differentiation w.r.t. τ, c is the total mass, $k_1, k_3 << 1$ and $(y, z) = (0, c)$ is the unique equilibrium.

- System (2) is a **multi-parameter singular perturbation problem** leading to three different scaling regimes: R_1 ($k_1 >> k_3$), R_2 ($k_1 \approx k_3$) and R_3 ($k_1 << k_3$).
- The limiting problem ($k_1 = k_3 = 0$)

$$\begin{aligned}y' &= -y^2\\ z' &= y^2\end{aligned} \qquad (3)$$

is shown in Figure 3. The critical manifold S is given by the line $y = 0$.

- Note that S is not normally hyperbolic, i.e., points $(0, z)$ are nilpotent.

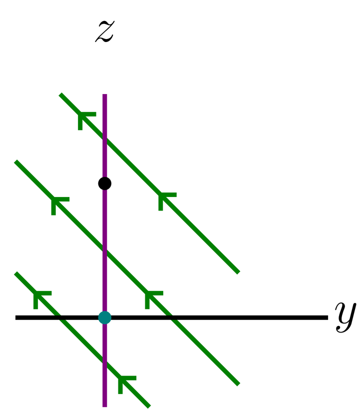

Figure 3: The non-hyperbolic critical manifold S and fast trajectories.

III. Scalings and Singular Limits

- To obtain a full description of (2) for small parameter values, we blow-up the origin of the parameter space by introducing

$$k_1 = r^2 \tilde{k}_1, \quad k_3 = r\tilde{k}_3 \qquad (4)$$

with $r \in [0, r_0)$ and $\tilde{k}_1 + \tilde{k}_3 = 1$.

- Add the equation $r' = 0$ to (2).
- Analyze the dynamics in two charts $\mathcal{K}_1$ and $\mathcal{K}_3$ corresponding formally to setting $\tilde{k}_1 = 1$ and $\tilde{k}_3 = 1$ in (4), respectively.

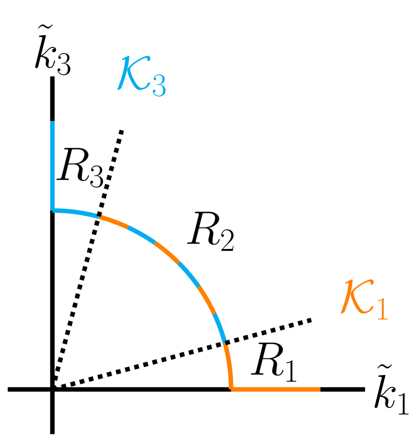

Figure 4: Parameter scaling regimes.

- In chart $\mathcal{K}_1$ system (2) is given by

$$\begin{aligned}y' &= r^2(c - y - z) - y^2 - r\tilde{k}_3 yz\\ z' &= y^2\\ r' &= 0.\end{aligned} \qquad (5)$$

- In chart $\mathcal{K}_3$ system (2) is given by

$$\begin{aligned}y' &= r^2\tilde{k}_1(c - y - z) - y^2 - ryz\\ z' &= y^2\\ r' &= 0.\end{aligned} \qquad (6)$$

- Although the limiting problems ($r = 0$) of (5) and (6) are identical in both charts, the regimes R_1, R_2 and R_3 have different asymptotics.
- If $\tilde{k}_1$ and $\tilde{k}_3$ are both bounded away from 0, i.e., in regime R_2, (5) and (6) are equivalent. Here we focus on R_2 (described in chart $\mathcal{K}_1$ for definiteness), which covers the choice of parameters in (1).

IV. Blow-up

- The non-hyperbolic critical manifold ($y = 0$, $r = 0$) of (5) is desingularized by a cylindrical blow-up, see Figure 5.
- The **blow-up** (cf. [1, 4]) is given by

$$\begin{aligned}\Phi : \mathbb{S}^1 \times \mathbb{R} \times [0, \rho_0] &\to \mathbb{R}^3\\ (\bar{y}, \bar{r}, \bar{z}, \rho) &\mapsto (\rho\bar{y}, \bar{z}, \rho\bar{r}).\end{aligned} \qquad (7)$$

- Note that $\mathbb{S}^1 \times \mathbb{R} \times \{0\}$ is the cylinder.
- In the scaling chart $\mathcal{K}_{12}$ ($\bar{r} = 1$) the blow-up is given by

$$y = \rho y_2,\ z = z_2,\ r = \rho.$$

- The equations in $\mathcal{K}_{12}$ are

$$\begin{aligned}y_2' &= c - \rho y_2 - z_2 - y_2^2 - \tilde{k}_3 y_2 z_2\\ z_2' &= \rho y_2^2\\ \rho' &= 0.\end{aligned} \qquad (8)$$

- System (8) is slow-fast in ρ. For $\rho = 0$, i.e., on the cylinder, we find a critical manifold S_1 given by

$$S_1 = \left\{ (y_2, z_2)^T \in \mathbb{R}^2 : z_2 = \frac{c - y_2^2}{1 + \tilde{k}_3 y_2} \right\},$$

which is normally attracting for $y_2 > \frac{-1}{\tilde{k}_3}$.

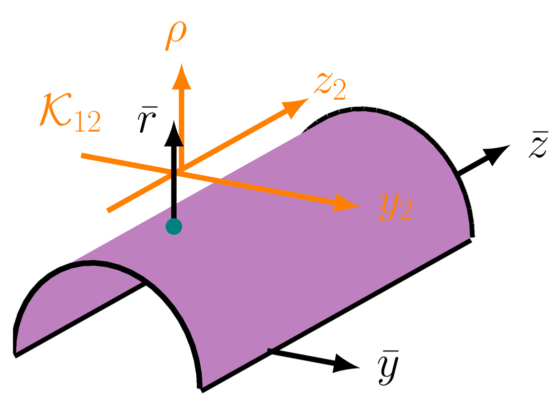

Figure 5: The preimage of the line $y = 0, r = 0$ under (7) is the cylinder $\rho = 0$.

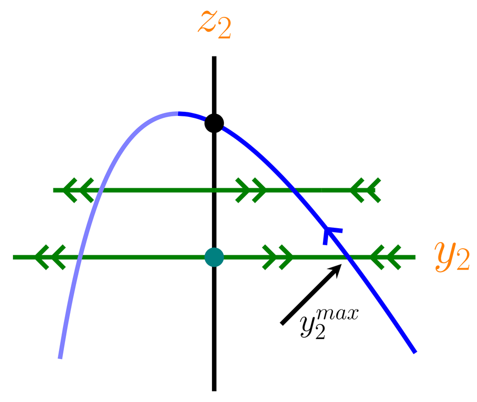

Figure 6: Dynamics of (8) with $\rho = 0$, i.e. on the cylinder for $\frac{1}{\tilde{k}_3^2} > c$.

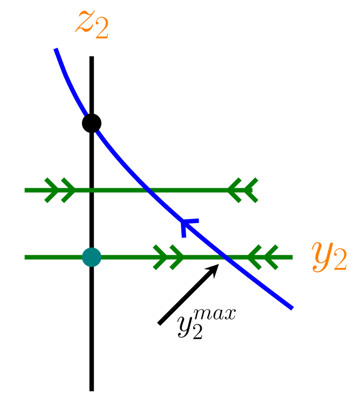

Figure 7: Dynamics of (8) with $\rho = 0$, i.e. on the cylinder for $\frac{1}{\tilde{k}_3^2} < c$.

V. Results

- There exists a singular orbit γ_0: A layer connecting the initial value to S_1, following the reduced flow on S_1 converging to the equilibrium.
- Fenichel theory [2] implies that there exists a smooth orbit γ_ρ close to γ_0, for $\rho > 0$ small enough.
- There is good quantitative agreement with the numerics:

$$y_{max}^{asy} = \sqrt{\frac{4}{3}} \cdot 10^{-\frac{9}{2}} + O(10^{-9}) \approx 3,6514 \cdot 10^{-5}.$$

- This proofs a heuristic argument in [3].

VI. Conclusion and Outlook

- Using (GSPT) and the blow-up method we obtained a **full asymptotic analysis** of the Robertson model in the regime R_2.
- We did not discuss the asymptotic behaviour in the regimes R_1 and R_3. These **more complicated** cases are part of ongoing work.
- Multi-parameter singular perturbations are expected to be important in many chemical reaction networks.

VII. References

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