A multi-parameter singular perturbation analysis of the Robertson model

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The Robertson model

Chemical reaction

1.	X	$\xrightarrow{k_1}$	Y
2.	$Y+Y$	$\xrightarrow{k_2}$	$Y+Z$
3.	$Y+Z$	$\xrightarrow{k_3}$	$X+Z$

Robertson model, H.H. Robertson 1966

$$\dot{x} = -k_1 x + k_3 yz$$
$$\dot{y} = k_1 x - k_2 y^2 - k_3 yz$$
$$\dot{z} = k_2 y^2$$

- With reaction rates $k_1 = 4 \cdot 10^{-2}$, $k_2 = 3 \cdot 10^{7}$, $k_3 = 10^4$ and initial value $(x_0, y_0, z_0)^T = (1, 0, 0)^T$.

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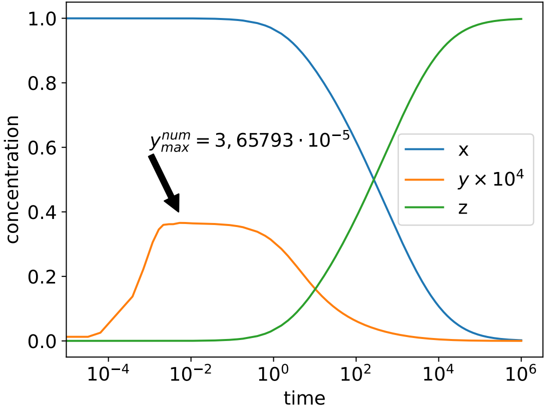
Why are we studying this model?

Numerics

- Dynamics on widely different time scales observed for $k_1, k_3 \ll k_2$.
- Note the logarithmic time scale!
- Numerically challenging to accurately describe all 3 phases of the reaction $\rightarrow$ used as a numerical test problem.
- Similar phenomena observed in many more complicated systems.



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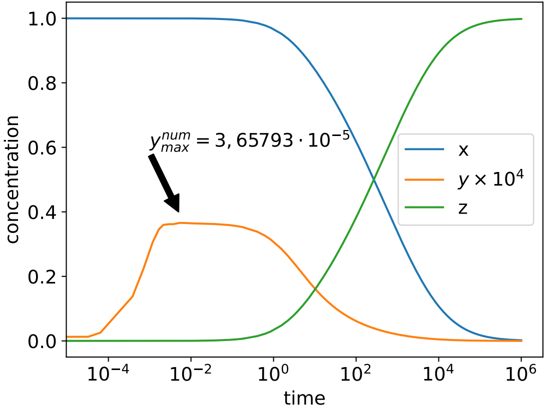
- **Today:** Asymptotic analysis based on geometric singular perturbation theory (GSPT).



GSPT 1

Fast variables $x \in \mathbb{R}^m$, slow variables $y \in \mathbb{R}^n$, $0 < \varepsilon \ll 1$.

Slow time scale t

$$\begin{cases} \varepsilon \dot{x} &= f(x, y, \varepsilon) \\ \dot{y} &= g(x, y, \varepsilon) \end{cases}$$

$$\overset{t = \tau\varepsilon}{\longleftrightarrow}$$

Fast time scale τ

$$\begin{cases} x' &= f(x, y, \varepsilon) \\ y' &= \varepsilon g(x, y, \varepsilon) \end{cases}$$

- For $\varepsilon > 0$ the two systems are equivalent.
- Two limiting problems for $\varepsilon = 0$:

Reduced problem

$$\begin{cases} 0 &= f(x, y, 0) \\ \dot{y} &= g(x, y, 0) \end{cases}$$

Layer problem

$$\begin{cases} x' &= f(x, y, 0) \\ y' &= 0 \end{cases}$$

GSPT 2

Reduced problem

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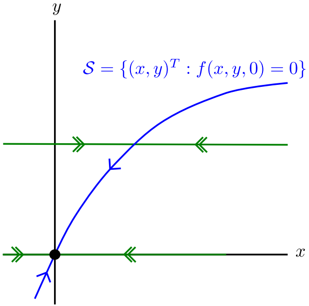
- Critical manifold
  $S := \{(x,y)^T : f(x,y,0) = 0\}$.



GSPT 2

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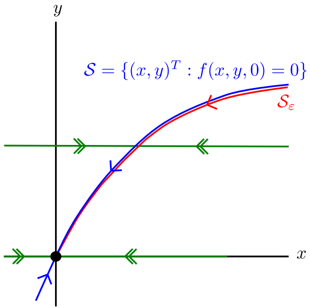
- Fenichel Theory (1979):
  If S satisfies some regularity conditions, then for $\varepsilon \ll 1$ it perturbs to invariant slow manifold S_ε, $\mathcal{O}(\varepsilon)$-close to S, with similar properties.



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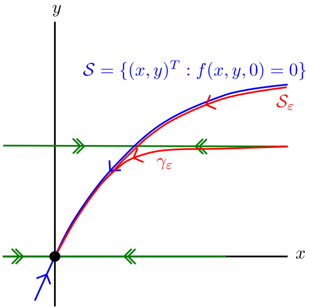


A two-parameter singular perturbation problem

- Initial value $(x_0, y_0, z_0) = (c, 0, 0)$ with $c > 0$.
- Use constant of motion $x(t) + y(t) + z(t) = c$ for all $t \geq 0$.

- New initial value $(y, z) = (0, 0)$ and equilibrium $(y, z) = (0, c)$
- Change to fast time scale $\tau = k_2 t$.
- Define new parameters:

$$\varepsilon_1 := k_1/k_2 \ll 1.$$
$$\varepsilon_2 := k_2/k_2 \ll 1.$$

Robertson model 3D

$$\dot{x} = -k_1 x + k_3 yz$$
$$\dot{y} = k_1 x - k_2 y^2 - k_3 yz$$
$$\dot{z} = k_2 y^2$$

$\downarrow$

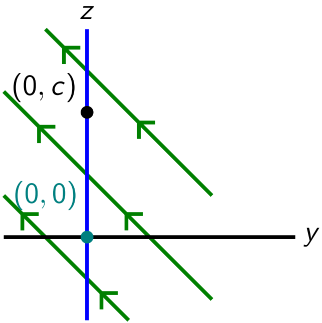
Robertson model 2D

$$y' = \varepsilon_1 (c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

A two-parameter singular perturbation problem

Limit problem $\varepsilon_1 = \varepsilon_2 = 0$:

- Very degenerate (double zero eigenvalue) line of equilibria $y = 0$.
- Contains the **initial value** and the **equilibrium**.



Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

Limit problem ($\varepsilon_1 = \varepsilon_2 = 0$)

$$y' = -y^2$$
$$z' = y^2$$

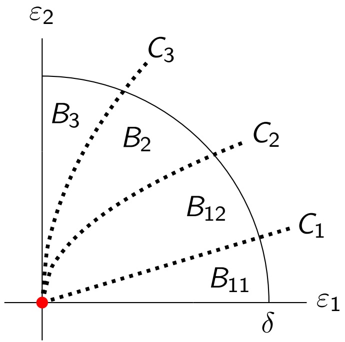
- Dynamics depends sensitively on $(\varepsilon_1, \varepsilon_2) \approx (0, 0)$!

Main Result

Theorem

1. In ${\varepsilon_1}^2 + {\varepsilon_2}^2 < \delta$, with $\delta > 0$, there exist four regions B_{11}, B_{12}, B_2, B_3 corresponding to different slow-fast structures.
2. In each of the regions $\exists$ a singular orbit γ_0 connecting the initial value $(0, 0)$ to the real equilibrium $(0, c)$.
3. The solution of the Robertson model converges to γ_0 in Hausdorff distance.

(B. and Szmolyan, 2024)



Parameter space

- Three regions B_1, B_2 and B_3 corresponding to

$$\varepsilon_2^2 \ll \varepsilon_1,\ \varepsilon_1 \approx \varepsilon_2^2,\ \varepsilon_1 \ll \varepsilon_2^2.$$

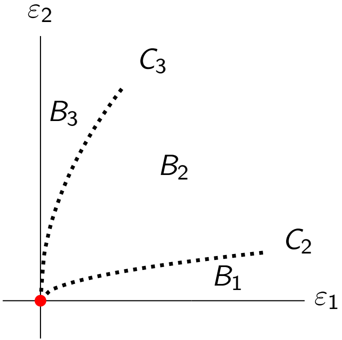
- Separated by the curves

$$C_2 := \{(\varepsilon_1, \varepsilon_2) \in \mathbb{R}^2 : \varepsilon_1 = \beta_2 \varepsilon_2^2\}$$

$$C_3 := \{(\varepsilon_1, \varepsilon_2) \in \mathbb{R}^2 : \varepsilon_1 = \beta_3 \varepsilon_2^2\}$$

  with $0 < \beta_3 < \beta_2$.

- GSPT not directly applicable to multi-parameter singular perturbations
  $\rightarrow$ describe parameter space in a suitable way (blow-up).

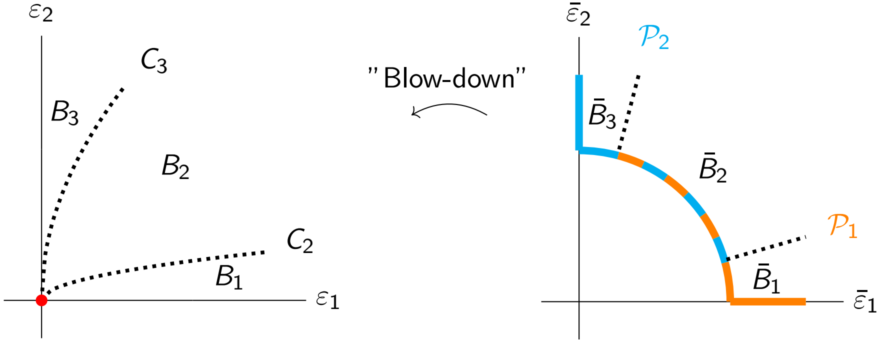


Blow-up of origin in parameter space

- The blow-up transformation is given by:

$$\varepsilon_1 = r^2\bar{\varepsilon}_1 \qquad \text{with } r \in [0,\infty) \text{ and } (\bar{\varepsilon}_1, \bar{\varepsilon}_2) \in S^1.$$
$$\varepsilon_2 = r\bar{\varepsilon}_2$$

- Analysis in directional charts $\mathcal{P}_1$ and $\mathcal{P}_2$ corresponding to $\bar{\varepsilon}_1 = 1$ and $\bar{\varepsilon}_2 = 1$.



Region B_2

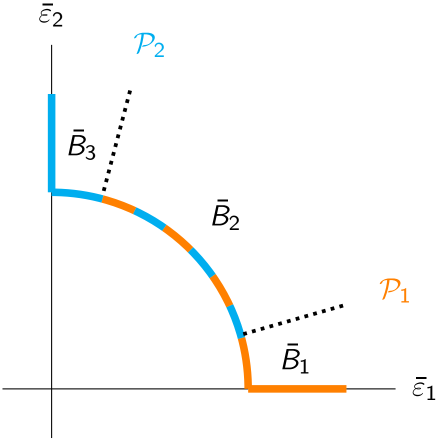
Robertson model 2D

$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

$\varepsilon_1 = r^2$, $\varepsilon_2 = r\tilde{\varepsilon}_2$,
rescaling $y = r\tilde{y}$

Chart $\mathcal{P}_1$, Region B_2 $\left(\tilde{\varepsilon}_2 \geq \sqrt{\frac{1}{\beta_2}}\right)$

$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2\tilde{y}z$$
$$z' = r\tilde{y}^2$$



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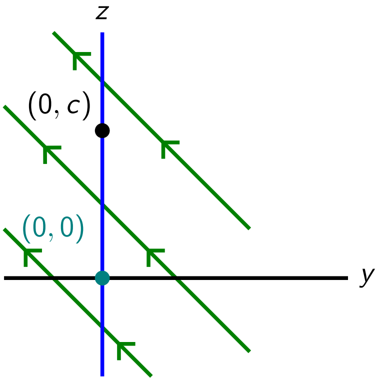


Region B_2

Chart $\mathcal{P}_1$, Region B_2 ($\tilde{\varepsilon}_2 \geq \sqrt{\frac{1}{\beta_2}}$)

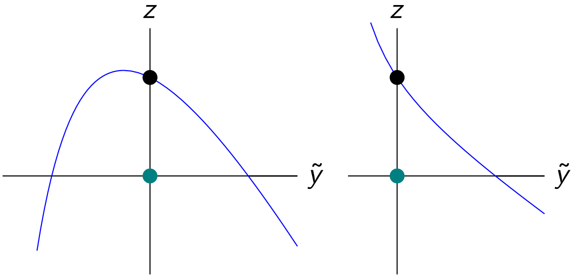
$$\tilde{y}' = c - r\tilde{y} - z - \tilde{y}^2 - \tilde{\varepsilon}_2\tilde{y}z$$
$$z' = r\tilde{y}^2$$

Layer problem (r=0)

$$\tilde{y}' = c - z - \tilde{y}^2 - \tilde{\varepsilon}_2\tilde{y}z$$
$$z' = 0$$

- Critical manifold:

$$\mathcal{S} = \left\{(\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{c-\tilde{y}^2}{1+\tilde{\varepsilon}_2\tilde{y}}\right\}$$



(a) $\frac{1}{\tilde{\varepsilon}_2^2} > c$. (b) $\frac{1}{\tilde{\varepsilon}_2^2} < c$.

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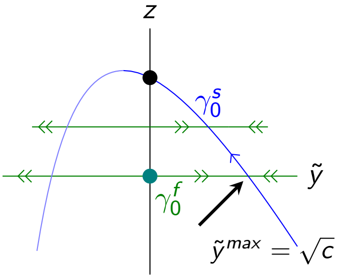
- $\mathcal{S}$ is normally attracting if $\tilde{y} > -\frac{1}{\tilde{\varepsilon}_2} + \sqrt{\frac{1}{\tilde{\varepsilon}_2^2} - c}$.
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.



Region B_2

Chart $\mathcal{P}_1$, Region B_2 ($\tilde{\varepsilon}_2 \geq \sqrt{\frac{1}{\beta_2}}$)

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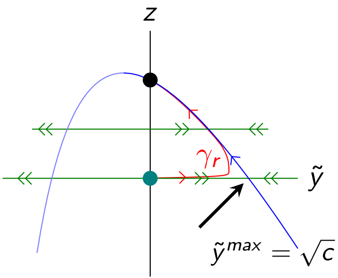
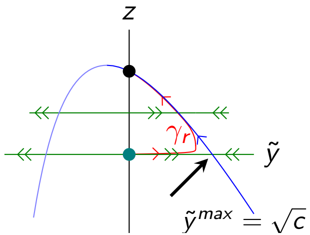
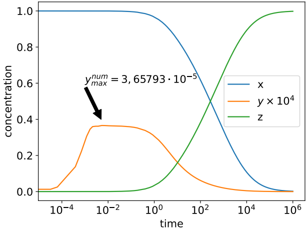
- Singular orbit $\gamma_0 := \gamma_0^f \cup \gamma_0^s$.
- Fenichel: $\exists\, r_0 > 0 \,\forall\, r \in (0, r_0]$ $\exists$ orbit γ_r, $\mathcal{O}(r)$-close to γ_0.



Comparison with Numerics

- Focus on the maximum of y along γ_r.
- Undoing all the rescalings:
  $y^{max} = \sqrt{\varepsilon_1}(\sqrt{c} + \mathcal{O}(\sqrt{\varepsilon_1})) = \sqrt{\varepsilon_1 c} + \mathcal{O}(\varepsilon_1)$.
- Inserting parameter values of the Robertson model:
  $y^{max} = 3,651 \cdot 10^{-5} + \mathcal{O}(10^{-9})$.
- Compare with $y_{max}^{num} = 3,65793 \cdot 10^{-5}$.





Region B_3

Robertson model 2D

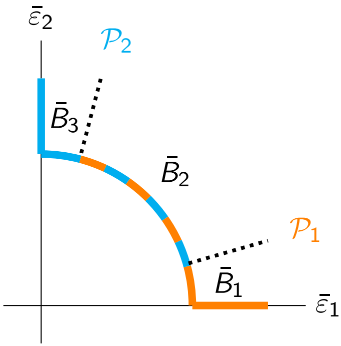
$$y' = \varepsilon_1(c - y - z) - y^2 - \varepsilon_2 yz$$
$$z' = y^2$$

$$\varepsilon_1 = r^2\tilde{\varepsilon}_1, \ \varepsilon_2 = r,$$

rescaling $y = r\tilde{y}$

Chart $\mathcal{P}_2$, Region B_3 $(\tilde{\varepsilon}_1 \leq \beta_3)$

$$\tilde{y}' = \tilde{\varepsilon}_1(c - r\tilde{y} - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = r\tilde{y}^2$$



Region B_3

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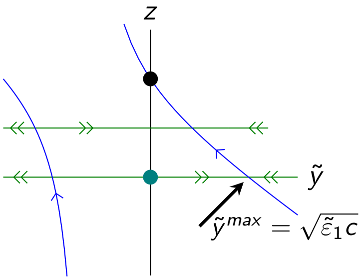
Layer problem (r=0)

$$\tilde{y}' = \tilde{\varepsilon}_1(c - z) - \tilde{y}^2 - \tilde{y}z$$
$$z' = 0$$

Critical manifold:

$$\mathcal{S} = \left\{(\tilde{y}, z)^T \in \mathbb{R}^2 : z = \frac{\tilde{\varepsilon}_1 c - \tilde{y}^2}{\tilde{\varepsilon}_1 + \tilde{y}}\right\}$$



(a) $\tilde{\varepsilon}_1 > 0$.

Region B_3

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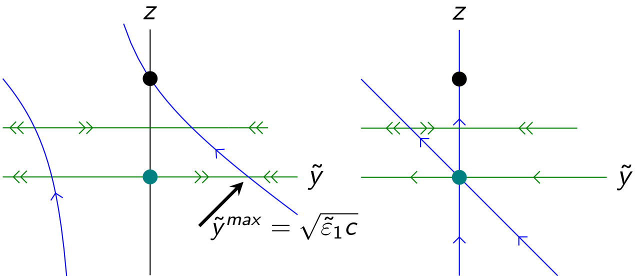


(a) $\tilde{\varepsilon}_1 > 0$. (b) $\tilde{\varepsilon}_1 = 0$.

Critical manifold $\mathcal{S}$ not normally hyperbolic at the origin for $\tilde{\varepsilon}_1 = 0$.
$\rightarrow$ Blow-up of the point $(\tilde{y}, z, \tilde{\varepsilon}_1) = (0, 0, 0)$ to a sphere.

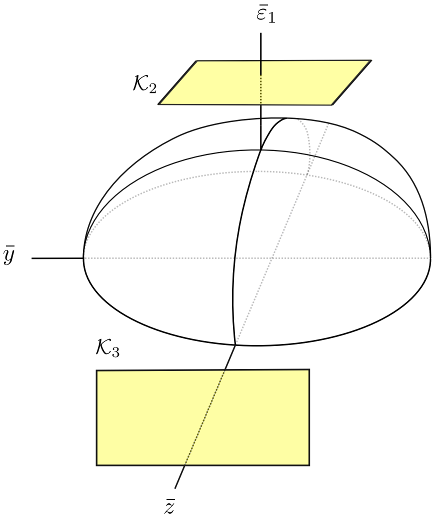
Blow-up of the origin

- Blow-up transformation:

$$\tilde{y} = \sigma \bar{y}$$
$$z = \sigma \bar{z}$$
$$\tilde{\varepsilon}_1 = \sigma^2 \bar{\varepsilon}_1$$

  with $\sigma \in [0, \infty)$ and $(\bar{y}, \bar{z}, \bar{\varepsilon}_1) \in S^2$.

- Pre-image of the origin is a sphere.
- Think of weighted polar coordinates.
- Analysis done in directional charts $\mathcal{K}_2$ and $\mathcal{K}_3$ corresponding to $\bar{\varepsilon}_1 = 1$ and $\bar{z} = 1$.



Dynamics in charts

$\mathcal{K}_2 : y = \sigma_2 y_2, \quad z = \sigma_2 z_2, \quad \tilde{\varepsilon}_1 = \sigma_2^2$

Dynamics in $\mathcal{K}_2$

$$\begin{aligned} y_2' &= c - \sigma_2 z_2 - y_2^2 - y_2 z_2 - r\sigma_2 y_2 \\ z_2' &= r y_2^2 \\ \sigma_2' &= 0. \end{aligned}$$

- Standard slow-fast with parameter r.
- Attracting critical manifold $S_2^a : \; y_2 = -\frac{z_2}{2} + \sqrt{\frac{z_2^2}{4} + c - \sigma_2 z_2}$.

$\mathcal{K}_3 : y = \sigma_3 y_3, \quad z = \sigma_3, \quad \tilde{\varepsilon}_1 = \sigma_3^2 \varepsilon_{13}$

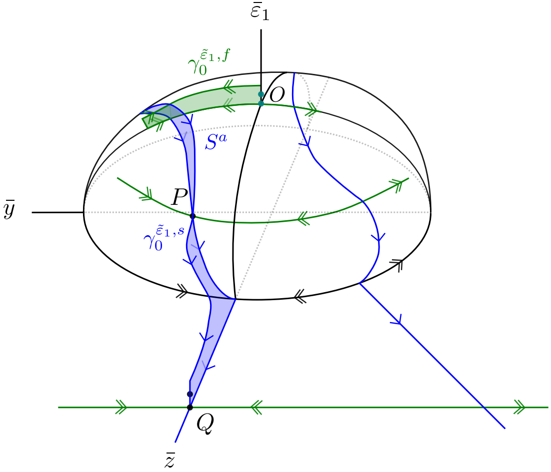
Dynamics in $\mathcal{K}_3$

$$\begin{aligned} y_3' &= \varepsilon_{13}(c - r\sigma_3 y_3 - \sigma_3) - y_3^2 - y_3 - r y_3^3 \\ \sigma_3' &= r\sigma_3 y_3^2 \\ \varepsilon_{13}' &= -2r\varepsilon_{13} y_3^2. \end{aligned}$$

- Standard slow-fast with parameter r.
- Attracting critical manifold $S_3^a : \; y_3 = -\frac{1}{2} + \sqrt{\frac{1}{4} + \varepsilon_{13}(c - \sigma_3)}$.

Desingularized dynamics

- The constants of motion $\tilde{\varepsilon}_1 = \sigma_2^2$ and $\tilde{\varepsilon}_1 = \sigma_3^2 \varepsilon_{13}$ let us control the reduced flow on the critical manifold S^a.
- For $\tilde{\varepsilon}_1 \in (0, \beta_3]$, we identify a singular orbit $\gamma_0^{\tilde{\varepsilon}_1} = \gamma_0^{\tilde{\varepsilon}_1, f} \cup \gamma_0^{\tilde{\varepsilon}_1, s}$, connecting the initial value $O = (0, 0, \tilde{\varepsilon}_1)^T$, via P, with the real equilibrium $Q = (0, c, \tilde{\varepsilon}_1)^T$.



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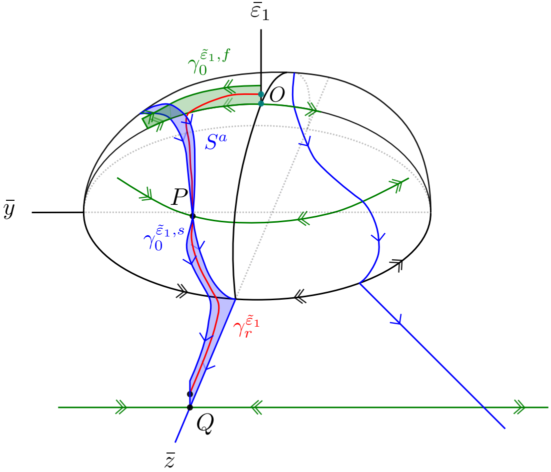
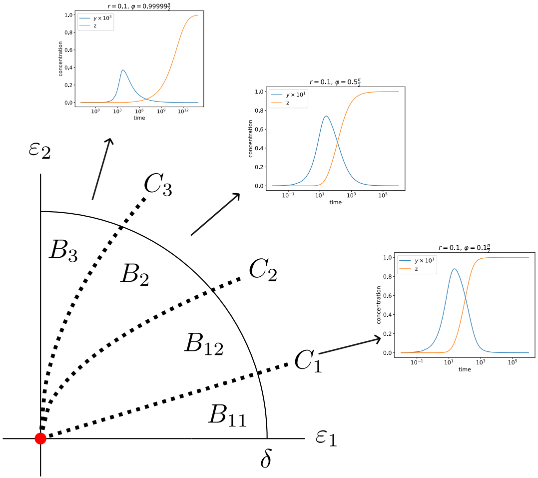
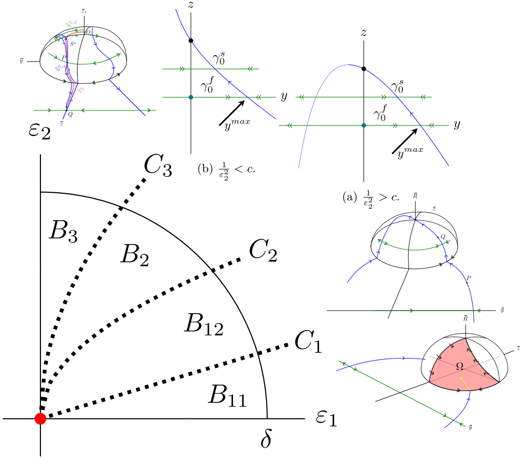
- S^a is normally attracting $\implies \exists$ perturbed orbit $\gamma_r^{\tilde{\varepsilon}_1}$ for r small enough.



Summary and Outlook





Summary and Outlook

- Full asymptotic analysis of the Robertson model under the assumption $k_1, k_3 \ll k_2$.
- Good qualitative and quantitative agreement with the numerics.
- A combination of blow-ups in parameter- and variable space makes GSPT applicable also in multi-parameter singular perturbations.
- Study more complicated multi-parameter singular perturbation problems.