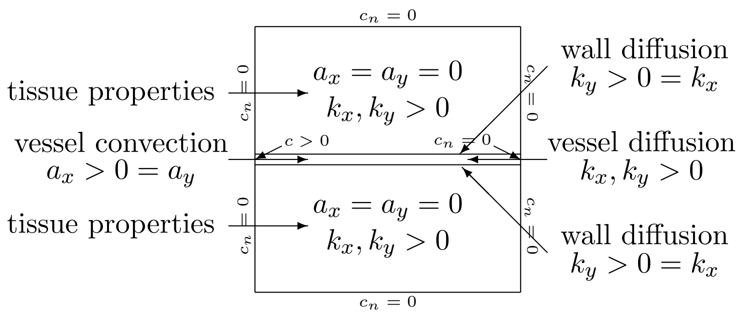
Mathematical Modelling in the Natural Sciences
SS21, Exercise Sheet 5

1. Write a Matlab code to simulate the convection and diffusion of contrast agent in a spatial domain $\Omega = (0,1)^2$ containing a single vessel according to

$$\left\{\begin{array}{rcll} \partial_t c + \partial_x(a_x c) + \partial_y(a_y c) &=& \partial_x(k_x \partial_x c) + \partial_y(k_y \partial_y c) & \\ &+& a_x \delta(x-0)\delta(y-\frac{1}{2})(c - c_0), & (x,y) \in \Omega, \quad t > 0 \\ \partial_n c &=& 0, & (x,y) \in \partial\Omega, \quad t > 0 \\ c &=& 0, & (x,y) \in \Omega, \quad t = 0 \end{array}\right.$$

   which is illustrated as follows:



   Here, blood flows through the vessel in the x-direction from left to right with convection coefficients $a_x > 0 = a_y$ and diffusion coefficients $k_x, k_y > 0$. In the tissue outside the vessel, there is no convection so $a_x = 0 = a_y$, but there is diffusion with diffusion coefficients $k_x, k_y > 0$. There is also diffusion over the boundary of the vessel in the y-direction with diffusion coefficients $k_y > 0 = k_x$. In general, the diffusion coefficients in the vessel, at the vessel wall and in the tissue outside the vessel are different. The boundary conditions for the concentration c are $c_n = 0$ on all sides. On the left side a constant inflow concentration $c > 0$ holds impulsively at the vessel inflow.

2. Let $c^\star$ be the solution to the previous problem using known values $a_x^\star, k_x^\star, k_y^\star$ in the vessel, $k_y^\dagger$ at the vessel wall and $k_x^\ddagger, k_y^\ddagger$ in the tissue outside the vessel. Use a perturbation of $c^\star$ as data and write a Matlab code to estimate the known convection and diffusion parameters. For this, it is recommended to use the Matlab function `lsqnonlin`.

3. Verify that the convolution kernel $K(t)$ for each of the two problems on page 161 of the lecture notes is given in section 2 of this article.

4. As discussed on page 162 of the lecture notes, construct a simple example $(N_\epsilon, C_{\mathrm{AIF}}, E_\epsilon)$ satisfying $N_\epsilon = C_{\mathrm{AIF}} * E_\epsilon$ and $N_\epsilon = \mathcal{O}(\epsilon)$ while $E_\epsilon = \mathcal{O}(\epsilon^{-n})$ for some arbitrary $n \in \mathbb{N}$.

5. For $t \in [0, T]$, $T = 4$, let

$$\begin{array}{rcl} C_{\mathrm{AIF}}(t) &=& 20te^{-3t} \\ C_{\mathrm{T}}(t) &=& 5e^{-3t}[-5 + 4e^t + e^{2t} - 6t] \\ K(t) &=& e^{-t} + e^{-2t} \end{array}$$

For $N \in \mathbb{N}$, let $t_i = i\Delta t$, $i = 0, \ldots, N$, $\Delta t = T/N$, let $\boldsymbol{C}_{\mathrm{AIF}} = \{C_{\mathrm{AIF}}(t_i)\}_{i=1}^N$, $\boldsymbol{C}_{\mathrm{T}} = \{C_{\mathrm{T}}(t_i)\}_{i=1}^N$ and $\boldsymbol{K} = \{K(t_i)\}_{i=1}^N$. Then let $\tilde{\boldsymbol{C}}_{\mathrm{AIF}}$ and $\tilde{\boldsymbol{C}}_{\mathrm{T}}$ be perturbations of $\boldsymbol{C}_{\mathrm{AIF}}$ and $\boldsymbol{C}_{\mathrm{T}}$, respectively. For the estimation of $\boldsymbol{K}$, compare the method of truncated singular value decomposition of pages 163 – 165 in the lecture notes with the method of contrained exponentials of pages 167 – 168 in the lecture notes. The Matlab functions `svd` and `lsqlin` are useful for the respective tasks.