Numerical methods in chemistry. Exercises 3

Problem 1

Given suitably well-behaved functions f and g establish that

$$f * g = g * f,$$

where the convolution $f * g$ is defined as

$$f * g = \int_0^t f(\tau)g(t-\tau)d\tau.$$

Problem 2

Use the convolution theorem to establish

$$\mathcal{L}^{-1}\left\{\frac{F(s)}{s}\right\} = \int_0^t f(\tau)d\tau.$$

Problem 3

Find the following convolutions:

(a) $t * \cos t$,

(b) $t * t$,

(c) $\sin t * \sin t$.

Problem 4

Use the Laplace transform to solve the following "driven" differential equation:

$$\frac{dx}{dt} + 3x = e^{2t},\ x(0) = 1.$$

Problem 5

Consider the **consecutive reaction**

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

with the rate constants $k_1 \neq k_2$ and initial concentrations $[A]_0 = a_0$, $[B]_0 = [C]_0 = 0$. Let us denote the concentrations at time t as $a(t) := [A]_t$, $b(t) := [B]_t$, and $c(t) := [C]_t$. As you will learn in the course of Chemical Kinetics next spring, these concentrations satisfy the following system of ordinary differential equations (ODEs):

$$\begin{aligned}\dot{a}(t) &= -k_1 a(t),\\ \dot{b}(t) &= k_1 a(t) - k_2 b(t),\\ \dot{c}(t) &= k_2 b(t).\end{aligned}$$

Use the Laplace transform to solve this system of ODEs and find explicit expressions for the concentrations of A, B, and C at time t in terms of a_0, k_1, k_2, and t.
Hint: Instead of solving the three ODEs simultaneously as in class for the *reversible reaction*, you can use the so-called **sequential method**, which only requires solving a single ODE at a time: Since the first equation [for $a(t)$] is not coupled to the others, it can be solved by itself. Once you find an explicit solution for $a(t)$, you can substitute it into the second equation and obtain an equation for $b(t)$ alone. Finally, you can substitute the solution for $b(t)$ into the third equation and solve a single equation for $c(t)$.