

# 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)  $\sin t * \sin t$ .

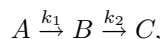
## Problem 4

Use the Laplace transform to solve the following “driven” differential equation:

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

## Problem 5

Consider the **consecutive reaction**



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  $c(t)$ .