CentraleSupelec **Numerical Methods, S8**

Project 1: The Belousov-Zhabotinskii reaction

In the context of chemical systems, an interesting but not well understood application concerns the chemical oscillators. In such systems, the composition can either reach a steady state or reach an oscillating regime, which leads to spatially and temporally evolving patterns such as in Fig. 1.

The Belousov-Zhabotinskii (BZ) reaction is one of these chemical oscillators. This reaction, discovered by Boris Belousov in the 1950s, can be initiated by mixing malonic acid, cerium(IV) sulfate, potassium bromate, and sulfuric acid: depending on the initial concentrations, the concentration of cerium(IV) and cerium(III) may oscillate because of the competition between the reduction of cerium(IV) into cerium(III) ions, which are in turn oxidized back into cerium(IV) because of bromate ions.

Figure 1: Spatial patterns generated by the Belousov-Zhabotinskii reaction in a Petri box.

In the literature, there is a lot of chemical mechanisms that have been proposed in order to model the BZ reaction. In the present project, we will investigated the Oregonator scheme. Using dimensionless form and a steady-state approximation, this scheme results in the following equation for the dimensionless concentration of Hypobromous acid x and cerium(IV) z:

$$\epsilon \frac{\mathrm{d}x}{\mathrm{d}t} = x(1-x) + f\frac{q-x}{q+x}z \tag{1}$$

$$\frac{\mathrm{d}z}{\mathrm{d}t} = x - z \tag{2}$$

where f is the stoechiometric coefficient, $q = 8 \times 10^{-4}$ is a combination of reaction constants, and ϵ a parameter that depends on the initial concentration of bromate and organic species.
The stoechiometric f depends on the composition of the organic species and may be between 0.4 and 1.0, whereas ϵ depends on the initial state and may be varied between 0.1 and 1.0. In the present project we focus on the values $f = 2/3$ and $\epsilon = 0.01$. The initial values are $x(t=0) = 0.5$ and $z(t=0) = 0.25$.

The objective of the present project is the following: as the system is oscillating, what are the minimum and maximum values reached by cerium (IV) (variable z)?