Mini-Projet: Traveling waves and spiral waves in excitable media: Belousov-Zhabotinsky

Students:

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1 Introduction

In this mini-projet, we focus on the analysis and simulation of traveling waves and spiral waves for the BZ reaction in excitable media. The objectives of the project are threefold: 1- to conduct an analysis similar to what we have done for the Nagumo equation in PC7, but for a stiffer problem, 2to analyze to what extent a splitting method can reproduce the dynamics of the wave when we want to use large time steps compared to the fastest scales in the system, 3- to study, depending on time, the dynamics in 2D of spiral waves along the line of [1].

2 Traveling waves for the BZ reaction in 1D

We are concerned with the numerical approximation of a model for the Belousov-Zhabotinski reaction, a catalyzed oxidation of an organic species by acid bromated ion (see [2] for more details and illustrations). We thus consider the model detailed in [4] and coming from the classic work of [3] which takes into account three species: hypobromous acid HBrO₂, bromide ions Br⁻, and cerium (IV). Denoting by a = [Ce(IV)], $b = [HBrO_2]$, and $c = [Br^-]$, we obtain a very stiff system of three PDEs:

$$\begin{cases}
\partial_t a - D_a \,\partial_x^2 a = \frac{1}{\mu} (-qa - ab + fc), \\
\partial_t b - D_b \,\partial_x^2 b = \frac{1}{\epsilon} (qa - ab + b(1 - b)), \\
\partial_t c - D_c \,\partial_x^2 c = b - c,
\end{cases} \tag{1}$$

 $x \in \mathbb{R}$, with diffusion coefficients D_a , D_b and D_c , and the real positive parameters: f, small q, and small ϵ and μ , such that $\mu \ll \epsilon \ll 1$.

The dynamical system associated with this system models reactive excitable media with a large time scale spectrum (see [4] for more details). The spatial configuration with the addition of diffusion develops propagating wavefronts with steep spatial gradients. Hence, this model presents all the difficulties associated with a stiff multi-scale configuration. The advantages of applying a splitting strategy to this problem have already been studied and presented in [1]. In what follows, we will briefly consider a 1D case of (1) in order to illustrate the errors of splitting schemes for stiff problems.

We consider then a 1D configuration of problem (1) with homogeneous Neumann boundary conditions and the following parameters, taken from [4]:

$$\epsilon = 10^{-2}, \qquad \mu = 10^{-5}, \qquad f = 3, \qquad q = 2 \times 10^{-4},$$
(2)

with diffusion coefficients:

$$D_a = 1/400, D_b = 1/400, D_c = 0.6/400, (3)$$

for a space region of [0,4]. Several level of sufficiently refined uniform mesh are considered while the exact solution T^s is approximated by a reference or *quasi-exact* solution T^s of the semi-discretized coupled reaction-diffusion problem (1), performed by Radau5 with very fine tolerances. The splitting schemes consider Radau5 and ROCK4 as integration methods for the reaction and diffusion problems.

- **2.1** Simulate the propagation of the wave in time. Show that there is a limit splitting time step for which the velocity of the wave is not predicted accurately any more.
- **2.2** Characterize the error for several splitting time steps and plot the error as a function of splitting time step.
- **2.3** Explain why this strategy can be considered as optimal in order to conduct a simulation of a traveling wave where stiffness is present at several levels.

3 Traveling waves for the BZ reaction in 2D

Following, what has been done in [1, 5], propose a study of the 2D case in terms of simulation and splitting methods.

References

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