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

Students :
Advisers : Laurent François and Laurent Séries

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, 2- to 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 $HBrO_2$, bromide ions Br^-, and cerium (IV). Denoting by $a = [\mathrm{Ce(IV)}]$, $b = [\mathrm{HBrO_2}]$, and $c = [\mathrm{Br^-}]$, we obtain a very stiff system of three PDEs:

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

$x \in \mathbb{R}$, 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]:

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

with diffusion coefficients:

$$D_a = 1/400, \qquad D_b = 1/400, \qquad D_c = 0.6/400, \tag{3}$$

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 $\mathcal{T}^s$ 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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