Journal of Computational Physics 256 (2014) 806–823

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Finite volume element approximation of an inhomogeneous Brusselator model with cross-diffusion

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ARTICLE INFO

Article history:
Received 24 August 2012
Received in revised form 31 August 2013
Accepted 5 September 2013
Available online 13 September 2013

Keywords:
Finite volume element method
Brusselator model
Cross-diffusion effect
Spatial patterns

ABSTRACT

This paper is concerned with the study of pattern formation for an inhomogeneous Brusselator model with cross-diffusion, modeling an autocatalytic chemical reaction taking place in a three-dimensional domain. For the spatial discretization of the problem we develop a novel finite volume element (FVE) method associated to a piecewise linear finite element approximation of the cross-diffusion system. We study the main properties of the unique equilibrium of the related dynamical system. A rigorous linear stability analysis around the spatially homogeneous steady state is provided and we address in detail the formation of Turing patterns driven by the cross-diffusion effect. In addition we focus on the spatial accuracy of the FVE method, and a series of numerical simulations confirm the expected behavior of the solutions. In particular we show that, depending on the spatial dimension, the magnitude of the cross-diffusion influences the selection of spatial patterns.

1. Introduction

The theory of spatial patterns generation goes back to the pioneering work of Turing [46]. Essentially, one chemical, the activator, stimulated and enhanced the production of the other chemical, which, in turn, depleted or inhibited the formation of the activator. The so-called Turing mechanism of pattern formation is onset by a diffusion-induced instability around the homogeneous steady state, that is, the concentration of the species evolves from an initial near homogeneity into inhomogeneous spatial distributions. This typically occurs if the diffusion of the inhibitor is large enough in comparison to that of the activator. This phenomenon has been reported in the context of the chlorite-iodide-malonic acid (CIMA) reaction [12,35] (see also [15]). On the other hand, further experimental studies have demonstrated that the cross-diffusion effect can lead to the formation of spatial and spatiotemporal patterns (see e.g. [47]). This is an interesting phenomenon whose applications range from biochemical to physical and economical processes. Numerous investigations from the viewpoint of mathematical and numerical analysis deal with some aspects of these problems, mainly focusing on the one- or two-dimensional case. In [4], it is shown that the spatial dimension has an important influence on the Turing pattern behavior. In the case when the wavelength of the Turing pattern is sufficiently (at least two times) larger than the thickness of the medium, three-dimensional patterns can be simplified to two-dimensional patterns. Otherwise, the three-dimensional patterns may differ from the well studied two-dimensional case (see [28,30] and the references therein). In this paper we aim at studying to which extent the spatial dimension influences the pattern behavior. Our analysis differs from the one in [4] in that we considered Turing patterns affected/induced by cross-diffusion mechanisms. We will focus on an inhomogeneous Brusselator model (see e.g. [21,36]), here assuming the following form

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0021-9991/$ – see front matter
http://dx.doi.org/10.1016/j.jcp.2013.09.009

$$\begin{cases} \dfrac{\partial u_1}{\partial t} - \Delta(D_{11}u_1 + D_{12}u_2) = -(\beta+1)u_1 + u_1^2 u_2 + \alpha, & (x,t) \in \Omega_T, \\ \dfrac{\partial u_2}{\partial t} - \Delta(D_{21}u_1 + D_{22}u_2) = \beta u_1 - u_1^2 u_2, & (x,t) \in \Omega_T, \\ \dfrac{\partial u_1}{\partial \eta} = \dfrac{\partial u_2}{\partial \eta} = 0, & (x,t) \in \Sigma_T, \\ u_1(x,0) = \psi_1(x), \quad u_2(x,0) = \psi_2(x), & x \in \Omega, \end{cases} \tag{1.1}$$

where $\Omega_T := \Omega \times (0,T)$, $\Sigma_T := (\partial\Omega) \times (0,T)$ for a fixed $T > 0$. We take α and β as positive constants, whereas D_{11} and D_{22} are the self-diffusion coefficients. The term $\Delta(D_{ij}u_j) = \nabla \cdot (\nabla(D_{ij}u_j))$ takes into account the flux of u_i, $\nabla(D_{ij}u_j)$, induced by the gradient of species u_j. Likewise, D_{ij} is the cross-diffusion coefficient for $i \neq j$. This system arises in the mathematical modeling of an autocatalytic chemical interaction governed by the following reaction mechanism:

$$A \xrightarrow{k_1} X, \qquad B + X \xrightarrow{k_2} Y + D, \qquad 2X + Y \xrightarrow{k_3} 3X, \qquad X \xrightarrow{k_4} \text{Products}.$$

Here A and B are the major species, X and Y the intermediate species. The third step is autocatalytic. As in [9], after employing the following scaled variables

$$\alpha = \left(\frac{k_1^2 k_3}{k_4^3}\right)^{\frac{1}{2}} A, \qquad \beta = \left(\frac{k_2}{k_4}\right) B, \qquad u_1 = \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} X, \qquad u_2 = \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} Y, \qquad \bar{t} = k_4 t,$$

and dropping the bar on t, we find that the evolution of u_1 and u_2 is governed by the ODE system

$$\begin{cases} \dfrac{du_1}{dt} = -(\beta+1)u_1 + u_1^2 u_2 + \alpha, \\ \dfrac{du_2}{dt} = \beta u_1 - u_1^2 u_2. \end{cases} \tag{1.2}$$

By introducing the cross-diffusion effect as in [47], system (1.2) leads to (1.1). This system is a suitable prototype for the study of a larger class of reaction–diffusion systems. By means of a linearized stability analysis, we will first show that if the parameters satisfy the condition $\beta < \min\{1+\alpha^2, 1 + \frac{\alpha^2 D_{11} - 2\alpha\sqrt{D_{11}D_{22}}}{D_{22}}\}$, then the cross-diffusion effect gives rise to the formation of patterns. Then, we focus on the spatial structure of these patterns with the help of a series of numerical tests.

An important number of contributions have been proposed to treat systems like (1.1) from a numerical perspective, either considering or not the cross-diffusion effect (see [2,5,6,8,14,18,21,39] for finite differences, finite volumes, spectral and finite element methods for the spatial discretization). Here, and following [11,27,37], we propose a new finite volume element (FVE) method for the numerical approximation of the underlying reaction–cross-diffusion system. We do not intend to carry out a thorough comparison of the performances of the different discretization strategies, but we rather introduce a FVE formulation because of its natural mass conservation property, and we employ it to study the formation and identification of spatial patterns.

FVE methods exhibit several advantages over some of the approaches mentioned above. These include the ability of treating arbitrarily complex geometries, unstructured and anisotropic meshes, a variety of boundary conditions (as robust finite element methods) and they feature local conservation and front capturing properties inherent mainly to finite volume methods (and highly desirable in the simulation of population dynamics). The key idea is that a complementary dual (or adjoint) mesh is introduced and a transfer map permits to rewrite a classical Galerkin formulation as a finite volume method (that is, in terms of fluxes passing through the faces of the primal elements). In the end, it is possible to reformulate the discrete problem as a Petrov–Galerkin problem. Related variants are also known as marker and cell methods [20], generalized difference methods [29], finite volume methods [1], covolume methods [34], box methods [3] or combined finite volume-finite element methods [24]. These are in general restricted to the two-dimensional case. We stress that even if in the present contribution we propose a FVE method for the particular inhomogeneous Brusselator system (1.1), the derivation of the FVE formulation is suitable for a larger class of Turing-type models including e.g. the well-known Gray–Scott [22], Gierer–Meinhardt [19] or the Schnakenberg [41] equations. In addition, the convergence properties of FVE methods can be studied rather straightforwardly by recasting the discrete formulation in a classical abstract framework for nonlinear Petrov–Galerkin problems. Even if a rigorous convergence analysis goes beyond the scope of the paper, we stress that optimal experimental rates of convergence are observed for both species, in the sense that the observed errors exhibit the same convergence order as the finite element interpolation operators.

The remainder of this paper is structured as follows. In Section 2 we deduce from the mathematical standpoint, the role of cross-diffusion in the generation of spatial patterns, and we provide the conditions for these patterns to appear. A FVE formulation for approximating the governing equations is detailed in Section 3, and some numerical tests including the study of convergence and formation of spatial patterns are shown in Section 4. Finally, some conclusions are drawn in Section 5. Proofs of our main results are collected in Appendices A, B and C.