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On the efficacy of a control volume finite element method for the capture of patterns for a volume-filling chemotaxis model

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ABSTRACT

In this paper, a *control volume finite element scheme* for the capture of spatial patterns for a volume-filling chemotaxis model is proposed and analyzed. The diffusion term, which generally involves an anisotropic and heterogeneous diffusion tensor, is discretized by piecewise linear conforming triangular finite elements (P1-FEM). The other terms are discretized by means of an upstream finite volume scheme on a dual mesh, where the dual volumes are constructed around the vertices of each element of the original mesh. The scheme ensures the validity of the discrete maximum principle under the assumption that the transmissibility coefficients are nonnegative. The convergence analysis is based on the establishment of a priori estimates on the cell density, these estimates lead to some compactness arguments in L^2 based on the use of the Kolmogorov compactness theorem. Finally, we show some numerical results to illustrate the effectiveness of the scheme to capture the pattern formation for the mathematical model.

1. Introduction

Patterns are the solutions of a reaction–diffusion system which are stable in time and stationary inhomogeneous in space, while pattern formation in mathematics refers to the process that, by changing a bifurcation parameter, the spatially homogeneous steady states lose stability to spatially inhomogeneous perturbations, and stable inhomogeneous solutions arise.

The pattern formation has been successfully applied to bacteria (see e.g. [1]) where we investigate specific and necessary parameters to obtain stationary distribution of the disease. Also, it has been applied to skin pigmentation patterns [2] to understand the diversity of patterns on the animal coat pattern, and many other examples.

The pattern formation depends on two key properties: the first is to apply the seminal idea of Turing [3] for a reaction–diffusion system and consequently determine the bifurcation parameters for the generation of stationary inhomogeneous spatial patterns (also called Turing Patterns), and the second is to apply a robust scheme to numerically investigate and capture the generation of spatio-temporal patterns. One of the most popular reaction–diffusion systems that can generate spatial patterns is the chemotaxis model.

Chemotaxis is the feature movement of a cell along a chemical concentration gradient either towards the chemical stimulus, and in this case the chemical is called chemoattractant, or away from the chemical stimulus and then the chemical is called chemorepellent. The mathematical analysis of chemotaxis models shows a plenitude of spatial patterns such as the chemotaxis models applied to skin pigmentation patterns [4,5]—that lead to aggregations of one type of pigment cell into a striped spatial pattern. Other models have been successfully applied to the aggregation patterns in an epidemic disease [6],

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tumor growth [7], angiogenesis in tumor progression [8], and many other examples. Theoretical and mathematical modeling of chemotaxis dates to the pioneering works of Patlak in the 1950s [9] and Keller and Segel in the 1970s [10,11]. The review article by Horstmann [12] provides a detailed introduction into the mathematics of the Keller–Segel model for chemotaxis.

In this paper, we present and study a numerical scheme for the capture of spatial patterns for a nonlinear degenerate volume-filling chemotaxis model over a general mesh, and with inhomogeneous and anisotropic diffusion tensors. Recently, the convergence analysis of a finite volume scheme for a degenerate chemotaxis model over a homogeneous domain has been studied by Andreianov et al. [13], where the diffusion tensor is considered to be proportional to the identity matrix, and the mesh used for the space discretization is assumed to be admissible in the sense of satisfying the orthogonality condition as in [14]. The upwind finite volume method used for the discretization of the convective term ensures stability and is extremely robust and computationally inexpensive. However, standard finite volume scheme does not permit handling anisotropic diffusion on general meshes, even if the orthogonality condition is satisfied. The reason for this is that there is no straightforward way to apply the finite volume scheme to problems with full diffusion tensors. Various "multi-point" schemes, where the approximation of the flux through an edge involves several scalar unknowns, have been proposed, see for e.g. [15,16] for the so-called SUCHI scheme, [17,18] for the so-called gradient scheme, and [19] for the development of the so-called DDFV schemes.

To handle the discretization of the anisotropic diffusion, it is well-known that the finite element method allows for an easy discretization of the diffusion term with a full tensor. However, it is well-established that numerical instabilities may arise in the convection-dominated case. To avoid these instabilities, the theoretical analysis of the *control volume finite element method* has been carried out for the case of degenerate parabolic problems with full diffusion tensors. Schemes with mixed conforming piecewise linear finite elements on triangles for the diffusion term and finite volumes on dual elements were proposed and studied in [20–24] for fluid mechanics equations, are indeed quite efficient.

Afif and Amaziane analyzed in [23] the convergence of a vertex-centered finite volume scheme for a nonlinear and degenerate convection–diffusion equation modeling a flow in porous media and without reaction term. This scheme consists of a discretization of the Laplacian by the piecewise linear conforming finite element method (see also [25,26]), the effectiveness of this scheme was tested in benchmarks of FVCA series of conferences [27]. Cariaga et al. in [24] considered the same scheme for a reaction–diffusion–convection system, where the velocity of the fluid flow is considered to be constant in the convective term.

The intention of this paper is to extend the ideas of [13,23,24] to a fully nonlinear degenerate parabolic systems modeling the effect of volume-filling for chemotaxis. In order to discretize this class of systems, we discretize the diffusion term by means of piecewise linear conforming finite element. The other terms are discretized by means of a finite volume scheme on a dual mesh (Donald mesh), with an upwind discretization of the numerical flux of the convective term to ensure the stability and the maximum principle of the scheme, where the dual mesh is constructed around the vertex of every triangle of the primary mesh.

The rest of this paper is organized as follows. In Section 2, we introduce the chemotaxis model based on realistic biological assumptions, which incorporates the effect of volume-filling mechanism and leads to a nonlinear degenerate parabolic system. In Section 3, we derive the *control volume finite element scheme*, where an upwind finite volume scheme is used for the approximation of the convective term, and a standard P1-finite element method is used for the diffusive term. In Section 4, by assuming that the transmissibility coefficients are nonnegative, we prove the maximum principle and give the *a priori* estimates on the discrete solutions. In Section 5, we show the compactness of the set of discrete solutions by deriving estimates on difference of time and space translates for the approximate solutions. Next, in Section 6, using the Kolmogorov relative compactness theorem, we prove the convergence of a sequence of the approximate solutions, and we identify the limits of the discrete solutions as weak solutions of the parabolic system proposed in Section 2. In the last section, we present some numerical simulations to capture the generation of spatial patterns for the volume-filling chemotaxis model with different tensors. These numerical simulations are obtained with our *control volume finite element scheme*.

2. Volume-filling chemotaxis model

We are interested in the *control volume finite element scheme* for a nonlinear, degenerate parabolic system formed by convection–diffusion–reaction equations. This system is complemented with homogeneous zero flux boundary conditions, which correspond to the physical behavior of the cells and the chemoattractant. The modified Keller–Segel system that we consider here, is very similar to that of Andreianov et al. [13], to which we have added tensors for the diffusion terms. Specifically, we consider the following system:

$$\begin{cases} \partial_t u - \operatorname{div}\left(\Lambda(x)\, a(u)\, \nabla u - \Lambda(x)\, \chi(u)\, \nabla v\right) = f(u) & \text{in } Q_T, \\ \partial_t v - \operatorname{div}\left(D(x)\, \nabla v\right) = g(u, v) & \text{in } Q_T, \end{cases} \tag{2.1}$$

with the boundary conditions on $\Sigma_T := \partial\Omega \times (0, T)$ given by

$$\left(\Lambda(x)\, a(u)\, \nabla u - \Lambda(x)\, \chi(u)\, \nabla v\right) \cdot \eta = 0, \qquad D(x)\, \nabla v \cdot \eta = 0, \tag{2.2}$$

and the initial conditions given by:

$$u(x, 0) = u_0(x), \qquad v(x, 0) = v_0(x), \quad x \in \Omega. \tag{2.3}$$