Journal of Computational and Applied Mathematics 239 (2013) 290–303

Contents lists available at SciVerse ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

A positivity-preserving finite element method for chemotaxis problems in 3D

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ARTICLE INFO

Article history:
Received 9 May 2011
Received in revised form 5 October 2011

Keywords:
Chemotaxis models
Flux limiters
Finite elements
Pattern formation
Bacteria aggregation

ABSTRACT

We present an implicit finite element method for a class of chemotaxis models in three spatial dimensions. The proposed algorithm is designed to maintain mass conservation and to guarantee positivity of the cell density. To enforce the discrete maximum principle, the standard Galerkin discretization is constrained using a local extremum diminishing flux limiter. To demonstrate the efficiency and robustness of this approach, we solve blow-up problems in a 3D chemostat domain. To give a flavor of more complex and realistic chemotactic applications, we investigate the pattern dynamics and aggregating behavior of the bacteria *Escherichia coli* and *Salmonella typhimurium*. The obtained numerical results are in good qualitative agreement with theoretical studies and experimental data reported in the literature.

1. Introduction

Chemotaxis, an oriented movement towards or away from regions of higher concentrations of chemical species, plays a vitally important role in the evolution of many living organisms. Experimental studies confirm that certain species (cells or bacteria) experience collective motion driven by attraction to or repulsion by other species (medicine, food, tumor angiogenic factor) [1]. The simplest mathematical description of chemotactic cell motion via a system of partial differential equations (PDEs) was proposed by Patlak [2], Keller and Segel [3,4]. Various extensions of their models have been used to analyze tumor angiogenesis and invasion [5,6], vasculogenesis [7], mesenchymal motion [8,9], biological pattern formation [10,11], multi-species chemotaxis with attraction and repulsion between competitive interacting species [12,13] etc. Besides the consideration of PDE models for chemotaxis there is also a scientific interest in chemotaxis models in the field of optimization algorithms by means of evolutionary concepts. Indeed Müller et al. [14] recently introduced an optimization algorithm based on bacteria chemotaxis. Therein, a main issue is the choice of a suitable chemosensitivity. Some of the aforementioned PDE models deal with alternative chemosensitivities which, therefore, may inspire improvements of the basic optimization algorithm by Müller et al.

From the mathematical point of view, several interesting questions arise in the context of classical (also called *minimal*) chemotaxis PDE models (cf. Section 2 for a common formulation). In particular, unbounded aggregation of cells may give rise to singularities at accumulation points. This phenomenon is known as the *blow-up* effect. Theoretical studies have shown that solutions to the 1D minimal model cannot blow up (see, e.g., [15]). In two dimensions, the existence of blow-up solutions depends on the initial cell density u_0 and chemotactic sensitivity χ. It is known that a (bounded) solution exists globally

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doi:10.1016/j.cam.2012.09.041

in time if $\|u_0\|_{L^1(\Omega)} < 4\pi\chi^{-1}$ in the nonsymmetric case and $\|u_0\|_{L^1(\Omega)} < 8\pi\chi^{-1}$ in the presence of radial symmetry [16]. Otherwise, a blow-up occurs in finite or in infinite time. For detailed results on finite time blow-up and blow-up in infinite time for solutions of parabolic–elliptic and parabolic–parabolic chemotaxis models, we refer the reader to [17–20].

In three dimensions, the threshold for the blow-up effect may also depend on the initial cell density, on the form of the chemotactic sensitivity, and on other parameters (see, e.g., [21,22]). Perthame [23] showed for parabolic–elliptic chemotaxis model that there is a blow-up in finite time if $(\int_\Omega |x|^2 u_0(\boldsymbol{x})\, d\boldsymbol{x})^2 < C\|u_0\|^2_{L_1(\Omega)}$, where C is a small constant. For parabolic–parabolic chemotaxis models Horstmann and Winkler [24] studied conditions under which the solution of a chemotaxis system with a chemotactic sensitivity of the form $\chi = c\,u^\alpha$ (where c and α are some constants) remains bounded or blows up in finite or infinite time. Their results prove the existence of initial data that give rise to blow-up solutions of the classical chemotaxis model in a bounded domain $\Omega \subset \mathbb{R}^3$. The existence, uniqueness, and uniform-in-time boundedness of global classical solutions for a 3D chemotaxis–haptotaxis system were investigated by Tao and Wang [25].

Another interesting phenomenon is the fact that a homogeneous stationary solution may become unstable for large values of the sensitivity function $\chi(u)$ under some conditions on the reactive source term in the chemotactic growth system. Such instabilities may give rise to rapidly evolving transient solutions, forming patterns which are observed in biological experiments (see, e.g., [26,10,27]).

The wealth of the methods for the numerical solution of chemotaxis problems includes positivity-preserving finite volume and finite element schemes [28–30], fractional step algorithms based on operator splitting [31,32], interior penalty/discontinuous Galerkin methods [33,34], and cell-overcrowding prevention models [35–37]. However, special care is required when it comes to the numerical simulation of the blow-up phenomenon and pattern formation. Steep gradients, spikes, and propagating fronts may give rise to nonphysical oscillations if the numerical scheme is not guaranteed to satisfy the discrete maximum principle (DMP). As a result, the cell density may become negative. Moreover, the blow-up or instability of approximate solutions may occur for purely numerical reasons.

In the present paper, we employ a high-resolution finite element scheme which satisfies the discrete maximum principle for linear and multilinear approximations on unstructured meshes. This algorithm is labeled FEM-TVD since it is based on a multidimensional generalization of total variation diminishing schemes for 1D conservation laws [38,39]. The proposed methodology guarantees mass conservation and keeps the cell density nonnegative. Another objective of this paper is to perform a series of numerical experiments for chemotaxis problems in the three-dimensional case. Most numerical studies published to date are concerned with 2D simulations, whereas the numerical behavior of solutions in 3D remains largely unexplored.

The article is organized as follows. In Section 2, we provide the analytical background and theoretical results for chemotaxis models in 3D. In Section 3, we outline the FEM-TVD algorithm that we used in the numerical study to be presented in Section 4. We demonstrate that the FEM-TVD method is well-suited for numerical simulations of chemotaxis problems, even in situations when the pure Galerkin method fails. In Sections 4.2 and 4.3, we consider realistic chemotaxis models which describe the aggregation and proliferation of the bacteria *Escherichia coli* and *Salmonella typhimurium*. Section 5 summarizes the pros and cons of the proposed approach.

2. Analytical background and theoretical results for chemotaxis models in 3D

The generic form of the chemotaxis problem to be solved in a three-dimensional domain $\Omega \subset \mathbb{R}^3$ reads

$$u_t = \nabla\cdot(D(u)\nabla u - A(u)\,B(c)\,C(\nabla c)) + q(u) \quad \text{in } \Omega, \tag{1}$$

$$c_t = d\Delta c - s(u)\,c + g(u)\,u \quad \text{in } \Omega, \tag{2}$$

where $u(t,\boldsymbol{x})$ denotes the cell density and $c(t,\boldsymbol{x})$ is the chemoattractant concentration. A particular model is defined by the formulas for the generic coefficients $D(\cdot), A(\cdot), B(\cdot), C(\cdot), q(\cdot), d, s(\cdot), g(\cdot)$. The above transport equation for u and reaction–diffusion equation for c are endowed with the initial conditions

$$u|_{t=0} = u_0, \qquad c|_{t=0} = c_0 \quad \text{in } \Omega. \tag{3}$$

It is common to prescribe the homogeneous Neumann boundary conditions

$$\boldsymbol{n}\cdot\nabla u = 0 \qquad \boldsymbol{n}\cdot\nabla c = 0 \quad \text{on } \Gamma, \tag{4}$$

or total flux boundary conditions of the form

$$\boldsymbol{n}\cdot(D(u)\,\nabla u - A(u)\,B(c)\,C(\nabla c)) = 0, \qquad \boldsymbol{n}\cdot\nabla c = 0 \quad \text{on } \Gamma, \tag{5}$$

where $\boldsymbol{n}$ is an outward normal to the boundary $\Gamma = \partial\Omega$.

The generic form (1)–(2) has also been described in [40] with slightly different notations. In this reference Hillen and Painter provided a summary over a number of variations of chemotaxis models like those considered in the current paper.

Before presenting a brief summary of the theoretical results for the above class of chemotaxis models, we cite a local existence result for the following problem

$$\left.\begin{array}{ll} u_t = \nabla(\nabla u - \chi(u,c)\nabla c) + f(u,c), & \boldsymbol{x}\in\Omega,\ t>0 \\ \tau c_t = \Delta c + g(u,c), & \boldsymbol{x}\in\Omega,\ t>0 \\ \boldsymbol{n}\cdot\nabla u = \boldsymbol{n}\cdot\nabla c = 0, & \boldsymbol{x}\in\Gamma,\ t>0 \\ u(0,\boldsymbol{x}) = u_0(\boldsymbol{x}), \qquad c(0,\boldsymbol{x}) = c_0(\boldsymbol{x}), & \boldsymbol{x}\in\Omega. \end{array}\right\} \tag{6}$$