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Nonnegativity of exact and numerical solutions of some chemotactic models☆

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ABSTRACT

We investigate nonnegativity of exact and numerical solutions to a generalized Keller–Segel model. This model includes the so-called "minimal" Keller–Segel model, but can cover more general chemistry. We use maximum principles and invariant sets to prove that all components of the solution of the generalized model are nonnegative. We then derive numerical methods, using finite element techniques, for the generalized Keller–Segel model. Adapting the ideas in our proof of nonnegativity of exact solutions to the discrete setting, we are able to show nonnegativity of discrete solutions from the numerical methods under certain standard assumptions. One of the numerical methods is then applied to the minimal Keller–Segel model. Recalling known results on the qualitative behavior of this model, we are able to choose parameters that yield convergence to a nonhomogeneous stationary solution. While proceeding to exhibit these stationary patterns, we also demonstrate how naive choices of numerical methods can give physically unrealistic solutions, thereby justifying the need to study positivity preserving methods.

1. Introduction

Negative approximations of intrinsically nonnegative quantities, such as density, are erroneous. They reduce confidence in simulation techniques, even when the negative values are close to zero. They often generate instabilities in nonlinear iterations thwarting convergence to a solution. Accordingly, nonnegativity of simulated solutions has become the first sanity check for any computer simulation of biological cell densities or chemical concentrations. However, not all nonlinear systems of partial differential equations come with a guarantee that their exact solutions are nonnegative. Their numerical discretization introduces a further layer of difficulty before one can certify that the simulated solution will be nonnegative. In this work, we examine these difficulties in the context of a specific class of nonlinear systems, which extend the influential chemotactic model proposed by Patlak [1] and later studied by Keller and Segel [2]. We provide a numerical approximation technique and prove that both the exact and the numerical solutions of the model are nonnegative.

We begin by describing a generalization of the Keller–Segel model that we shall focus on in later sections. It involves a species of density u occupying a domain $\Omega \subseteq \mathbb{R}^n$ and N reacting chemicals of concentrations v_i, $i = 1, 2, \ldots, N$, represented as components of a vector function $\vec{v}$. We are interested in the situation where one of these chemicals is a chemoattractant for

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the species. This situation is modeled by the following system of equations, taken from [3], which we refer to as a *generalized Keller–Segel system* throughout this paper:

$$\partial_t u = \nabla \cdot (D\nabla u - \chi u \nabla v_N) \quad x \in \Omega,\ t > 0, \tag{1a}$$

$$\partial_t \vec{v} = \tilde{D}\Delta\vec{v} + \vec{\alpha}u + \vec{g}(\vec{v}) \quad x \in \Omega,\ t > 0, \tag{1b}$$

$$u(x,0) = u_0(x), \qquad \vec{v}(x,0) = \vec{v}_0(x) \quad x \in \Omega, \tag{1c}$$

$$\frac{\partial u(x,t)}{\partial n} = \frac{\partial v_i(x,t)}{\partial n} = 0 \quad x \in \partial\Omega,\ t \geq 0,\ 1 \leq i \leq N. \tag{1d}$$

The rate of change of $\vec{v}$ is determined by a chemical reaction network, represented by the (nonlinear) function $\vec{g}(\vec{v})$. The parameter χ describes the chemotactic sensitivity. The term $\vec{\alpha}u$, with a constant vector $\vec{\alpha} \in \mathbb{R}^N$ satisfying $\vec{\alpha} \geq 0$, indicates that some or all of the chemicals can be produced by the species. (Here and throughout, the notation $\vec{w} \geq 0$ signifies that each component of $\vec{w}$ is nonnegative.) Above, we have augmented the differential equations with no-flux boundary conditions and initial conditions. We assume that the initial data $u_0 \geq 0$ and $\vec{v}_0 \geq 0$ are nontrivial functions on Ω. Additionally, $\vec{n}$ generically denotes the unit outward normal on the boundary of any domain under consideration and $\partial/\partial n = \vec{n} \cdot \vec{\nabla}$. (E.g., in (1), the domain under consideration is Ω and $\vec{n}$ is the outward unit normal on the boundary $\partial\Omega$.) For now, we assume that $\partial\Omega$ is Lipschitz so that $\vec{n}$ is defined a.e. on $\partial\Omega$, but we will place further assumptions on Ω in later sections for theoretical reasons. Throughout, we also use the abbreviated notations ∂_t and ∂_i for $\partial/\partial t$ and $\partial/\partial x_i$, respectively. We note that other generalizations of the Keller–Segel system have recently been proposed in [4,5], but most of their analysis is limited to a particular number of chemicals, and moreover their focus is not on the nonnegativity questions we intend to study here.

Let us now consider a few examples that fit the generalized Keller–Segel model (1).

Example 1.1 (*Minimal Keller–Segel Model*)**.** This very well-known nonlinear system of two equations is obtained by choosing, in (1),

$$N = 1, \qquad \vec{\alpha} = \begin{bmatrix}\alpha_1\end{bmatrix}, \qquad \vec{g}(\vec{v}) = \begin{bmatrix}-\gamma v_1\end{bmatrix},$$

with $\alpha_1 > 0$ and $\gamma > 0$. In this setting, u represents the density of the amoeba *Dictyostelium discoideum* and v the density of the chemoattractant cyclic adenosine monophosphate (cAMP). Keller and Segel proposed this model to understand aggregation by chemotaxis in [2]. The extensive reviews in [6,7] puts this model in perspective and points to many known results on the behavior of its solutions.

Example 1.2 (*Full Keller–Segel Model with Decay*)**.** The minimal Keller–Segel model from the previous example is a simplified version of a four-equation model, also originally derived in [2]. As in the case of the minimal model we let u denote the density of the amoeba, but the density of the cAMP is now denoted by v_3. Additionally, an enzyme which degrades the cAMP, and is also emitted by the amoeba, enters the model. We denote the density of this enzyme by v_1. As explained in [2] or [6], the cAMP and the enzyme undergo a reversible reaction to form a complex, with density v_2. (This complex may then degrade into the enzyme plus a degraded product which is not typically considered in this model.) The reactions just described can be briefly written as

$$v_1 + v_3 \longleftrightarrow v_2 \longrightarrow v_2 + \text{ degraded product}. \tag{2}$$

Moreover, we assume that the enzyme decays at some positive rate γ_1, as justified biologically in [8]. Assuming a linear (in u) chemotactic sensitivity function, as in the minimal model, as well as constant production rates, we can now express the four equation model in the setting of (1). If the forwards, backwards and decay reaction rate constants from (2) are given by k_i for $1 \leq i \leq 3$ respectively, using the laws of mass action, the reaction network is described by

$$\vec{g}(\vec{v}) = \begin{bmatrix} -k_1 v_1 v_3 + (k_2 + k_3) v_2 - \gamma_1 v_1 \\ -(k_2 + k_3) v_2 + k_1 v_1 v_3 \\ -k_1 v_1 v_3 + k_2 v_2 \end{bmatrix}.$$

Using this $\vec{g}$ in (1), and setting chemical production rates by

$$\alpha = \begin{bmatrix} \alpha_1 \\ 0 \\ \alpha_3 \end{bmatrix},$$

with $\alpha_1 > 0$ and $\alpha_3 > 0$, we obtain the "full Keller–Segel model". Except for the decay term, this is the same as the four-equation model of [2].

Example 1.3 (*Dimerization*)**.** The chemistry of dimerization involves two molecules of a chemical v_1 combining reversibly to form another chemical v_2. This reaction can be written as

$$2v_1 \longleftrightarrow v_2$$