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Partial-moment minimum-entropy models for kinetic chemotaxis equations in one and two dimensions

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ABSTRACT

The aim of this work is to investigate the application of partial moment approximations to kinetic chemotaxis equations in one and two spatial dimensions. Starting with a kinetic equation for the cell densities we apply a half-/quarter-moments method with different closure relations to derive macroscopic equations. Appropriate numerical schemes are presented as well as numerical results for several test cases. The resulting solutions are compared to kinetic reference solutions and solutions computed using a full moment method with a linear superposition strategy.

1. Introduction

The migration of cells is a complex process that is influenced by many factors such as external light, the pH or the oxygen concentration. In the following we concentrate on chemotaxis, the movement of cells in response to a chemical stimulus. A substance which causes cells to move in the direction of its gradient is called chemoattractant. The ideas of this work can easily be extended to chemorepellents, which have the opposite effect. Chemotaxis plays an important role in a lot of biological processes: It drives the movement of bacteria towards food and away from poisons or leads the sperm in the direction of the egg during fertilization. In multi-cellular organisms, it controls the guided accumulation of cells during embryological development and the movement of lymphocytes in the process of immunological response [1–3]. During cancer metastasis, mechanisms that allow chemotaxis can be subverted. Therefore a better understanding of the associated processes may lead to the development of novel therapeutic strategies. The movement of many bacteria, such as Escherichia coli which has been studied and described most intensely, is controlled by the alignment of their flagella, whip-shaped appendices with a rotary motor at their bases that are embedded in the cell membrane. Counter-clockwise rotation aligns the flagella, causing the bacterium to swim in a straight line ("run phase"); clockwise rotation causes the flagella to point in different directions, resulting in a movement on the spot ("tumble phase"). The latter re-orients the bacterium, so that overall we observe a random walk [4,5]. A chemical stimulus influences the motion in the following way: if receptors sense that the bacterium is moving in the direction of the chemoattractant gradient, the "run phase" will be extended; if the concentration of the chemoattractant is decreasing in the direction of movement, it will be shortened. This results in a biased random walk [2]. Consideration of additional effects on the chemoattractant, such as production by the bacteria themselves, decay and diffusion, further increases the complexity of the model.

The original equations to model chemotaxis are the Keller–Segel equations. These equations have been intensively investigated, see for example [6–9] for a phenomenological, [1,10,11,3] for a kinetic and micro–macro derivation, and [12–17] for a qualitative analysis of its solutions. For a survey and an extended reference list, see for example [10].

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Our starting point is the classical kinetic chemotaxis equation [2]. Scaling it with the so called diffusive scaling leads to the Keller–Segel equation, see [2]. In general, the derivation of Keller–Segel type models, including flux-limited diffusion models and Fokker–Planck type models, from underlying kinetic or microscopic models is discussed for example in [10,18,2]. In particular, using moment closure approaches one may obtain macroscopic equations intermediate between kinetic and Keller–Segel equations, see the above mentioned references or [19,7]. First order full moment equations with a linear closure function are sometimes called the Cattaneo equations. Applying maximum entropy closures one obtains improved first order full moment models [20]. Half- and quarter-moment closures have been developed for kinetic radiative transfer equations in [21,22]. It has been shown for these applications in various numerical experiments that the partial moment methods yield macroscopic models that can produce satisfying approximations. We refer to [21].

The aim of this work is to investigate the application of partial moment approximations to kinetic chemotaxis equations in one and two dimensions. Starting with a kinetic equation for the cell densities we apply a half- and quarter-moment method with varying closure relations to derive macroscopic equations in Section 2. By applying numerical schemes that use certain properties of the moment systems and implementing it using Matlab [23], we obtain numerical results for several different test cases. Moreover, we compare the results to kinetic reference solutions and solutions computed using a full moment method and a linear superposition strategy. This work should be seen as a first step towards an efficient simulation strategy for kinetic chemotaxis equations via further refinement of the sphere, leading from a quarter moment model to a general first-order partial-moment model, which will hopefully converge to the true kinetic solution with a small number of refinements. This strategy should yield similar results as higher order moment methods while being numerically much more efficient due to the inherent structure of the first order partial moment models.

2. Chemotaxis equations

The dynamics of chemotaxis can be modelled by the kinetic equations

$$\partial_t f + v \cdot \nabla_{\mathbf{x}} f = -\lambda(f - C_V \rho) + C_V \alpha \rho v \cdot \Phi(\nabla m), \tag{2.1}$$

$$\partial_t m - D_m \Delta_{\mathbf{x}} m = \beta \rho - \delta m, \tag{2.2}$$

where $f(t, \mathbf{x}, v)$ is the density of cells at time t and location $\mathbf{x} \in \mathbb{R}^d$, with velocity $v \in V$, whereas $\rho(t, \mathbf{x}) = \int_V f \, dv$ describes the overall density of cells at time t and location $\mathbf{x}$. $m(t, \mathbf{x})$ is the concentration of the chemoattractant at time t and location $\mathbf{x}$. V is the set of admissible velocities; since we assume that the cells move in arbitrary directions, but with constant speed, we have $V = S^2 = \{v \in \mathbb{R}^3 \mid \|v\|_2 = 1\}$ in three dimensions and consider the projections $V = [-1, 1]$ in one and $V = B_1(0) = \{v \in \mathbb{R}^2 \mid \|v\|_2 \leq 1\}$ in two dimensions [11]. The normalization constant C_V is determined by V: $C_V = \frac{1}{2}$ in one and $C_V = \frac{1}{4\pi}$ in two dimensions. The remaining coefficients characterize the biological system: λ and α describe the diffusivity and the chemotactic sensitivity of the cells. D_m is the diffusivity, β the production rate by the cells and δ the rate of chemical decay of the chemoattractant. The function Φ acts as a limiter for the influence of the chemoattractant gradient ∇m, which models the fact, that the "run phase" can only be extended to a certain extent. In the following we use

$$\Phi(\mathbf{x}) = \begin{cases} \left(\dfrac{\|\mathbf{x}\| - s}{\sqrt{1 + (\|\mathbf{x}\| - s)^2}} + s \right) \dfrac{\mathbf{x}}{\|\mathbf{x}\|} & \|\mathbf{x}\| \geq s, \\ \mathbf{x} & \|\mathbf{x}\| \leq s, \end{cases}$$

where the parameter $s \geq 0$ determines the extent of the limiting: $\max(\|\Phi(\mathbf{x})\|) \leq s + 1$. Using this limiter in our simulation prevents blow up of the solution in finite time [15].

Assuming that $\lambda \geq C_V \alpha (s + 1)$, the right-hand side of (2.1) can be written in the turning-kernel representation with non-negative kernel, which ensures that (2.1) admits a non-negative solution f [2].

We note that Eq. (2.1) is related via a diffusive scaling limit $t \to \epsilon^2 t$ and $\mathbf{x} \to \epsilon \mathbf{x}$ to a special case of the general Patlak–Keller–Segel

$$\partial_t \rho - \frac{1}{3\lambda} \Delta_{\mathbf{x}} \rho = -\frac{\alpha}{3\lambda} \nabla_{\mathbf{x}} \cdot (\rho \Phi(\nabla m)).$$

See [24] or [2] for details and rigorous proofs.

3. Moment models

In this section we introduce the method of moments and explore how it can be used to derive macroscopic equations from our kinetic equation (2.1). It can be seen as a Galerkin approximation in the velocity component v, by projecting the kinetic density $f(t, \mathbf{x}, v)$ in v onto a finite-dimensional subspace of $L_2(V, \mathbb{R})$. Assume that this subspace is spanned by the basis $\mathbf{b} : V \to \mathbb{R}^n$, moments of f are defined as

$$\mathbf{u}(t, \mathbf{x}) = \int_V \mathbf{b}(v) f(t, \mathbf{x}, v) \, dv =: \langle \mathbf{b} f \rangle,$$