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Coupled lattice Boltzmann method for generalized Keller–Segel chemotaxis model

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ABSTRACT

In this work, an efficient and stable lattice Boltzmann method (LBM) for generalized Keller–Segel (K–S) chemotaxis model is proposed. Through the Chapman–Enskog analysis, the proposed LBM can correctly recover to the K–S model. The stability of the proposed LBM has been improved through adding correction terms in the evolution equations. Moreover, a local computational scheme for the gradient operator, which is included in the evolution equation, is developed, making the proposed LBM be implemented locally. Hence, both 2D and 3D problems with arbitrary geometries can be processed easily. In the numerical experiments, several representative chemotaxis problems are studied, including the blow up problem in square and circle domains, two-species chemotaxis blow up problem, chemotactic bacteria pattern formation in semi-solid medium in circle domain, 3D pattern formation in liquid medium, and the tumor invasion into surrounding healthy tissue. The numerical results demonstrate the high efficiency, stability and robustness of the proposed LBM. Furthermore, the capability of the proposed LBM in handling both 2D and 3D problems with complex domain is also illustrated.

1. Introduction

The chemotaxis, which describes the movements of bacteria, biological cells and organisms in response to chemical gradients, widely exists in nature, and also plays a crucial fundamental role in a wide range of biological phenomena [1], such as bacteria/cell aggregation, complex pattern formation and the tumor cells invading surrounding environment. Understanding the behavior of bacteria/cell chemotaxis is of important significance to the medical and biological applications.

In the recent years, the chemotaxis has attracted great interest to both experimentalists and theoreticians. Many mathematical models have been developed to describe the chemotactic bacterial populations or cells behavior. The most generalized and widely utilized chemotaxis model is the Keller–Segel (K–S) model, which was originally proposed by Keller and Segel in modeling the movement of slime molds [2,3]. Thereafter, most of the subsequent chemotaxis models were developed based on the generalized K–S model, which is given by [4,5]

$$\frac{\partial b(\mathbf{x},t)}{\partial t} = \nabla\cdot(\mu(b,s)\nabla b(\mathbf{x},t) - \chi(b,s)b(\mathbf{x},t)\nabla s(\mathbf{x},t)) + g(b,s) - h(b,s), \tag{1a}$$

$$\frac{\partial s(\mathbf{x},t)}{\partial t} = D\nabla^2 s(\mathbf{x},t) - f(b,s), \tag{1b}$$

where $b(\mathbf{x},t)$ is the density of the bacterial population, $s(\mathbf{x},t)$ is the attractant concentration at spatial position $\mathbf{x}$ and time t, $\mu(b,s)$ is the bacterial diffusion coefficient, $\chi(b,s)$ is the chemotactic coefficient, $g(x,t)$ and $h(b,s)$ are functions describing

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cell growth and death, respectively, $f(b, s)$ is a function describing attractant degradation, and D is the diffusion coefficient of the attractant. More complicated and more realistic chemotaxis models can be extended by considering additional factors, such as more accurate terms describing production and uptake of the chemoattractant by cells, tumor angiogenesis and invasion [6,7], vasculogenesis [8], biological pattern formation [9,10], and multi-species chemotaxis with attraction and repulsion between competitive interacting species [11,12].

Due to the density dependent cross diffusion term, the chemotaxis model is a highly nonlinear coupled system. From mathematical point of view, it is very difficult to obtain analytical solution of the chemotaxis systems. Thus it is very desirable to develop numerical methods for modeling and analyzing chemotaxis systems. However, the solution of the chemotaxis model, which rapidly grows in small neighborhoods of concentration points/curves, may blow up or exhibit a very singular, spiky behavior. It brings great challenge to numerical methods to capture such singular solutions. Recently, a variety of numerical approaches for chemotaxis models have been developed, such as the finite volume, finite element schemes [13,14], fractional step algorithms based on operator splitting [15,16], interior penalty/discontinuous Galerkin methods [17,18], upwind-difference potentials method [19], and cell-overcrowding prevention models [20–22]. However, these methods are almost developed for a simple version of the K–S model. In Ref. [23], a second-order positivity preserving central-upwind scheme for a class of chemotaxis models and haptotaxis models was developed. But the scheme only considered two-dimensional problems and the computational domain is rectangular. In Ref. [19], Y. Epshteyn developed an upwind-difference potentials method which can handle complex geometry for the Patlak–Keller–Segel chemotaxis model, but this method is also for two-dimensional problems. From the above, an accurate, stable and efficient numerical method for generalized K–S model in handling both 2D and 3D problems with arbitrary geometries is needed.

In the past 20 years, the lattice Boltzmann method (LBM) has achieved great success in modeling complex physics in fluids due to its easy programming, intrinsical parallelism and the ability to incorporate complicated boundary conditions [24–27]. In the recent years, LBM also shows potentials to simulate nonlinear systems, such as reaction–diffusion equation [28–31], convection–diffusion equation [32–34] and Nernst–Planck equation [35] and so on. However, for the chemotaxis systems, only Hilpert [36] developed an LBM for the simplified bacterial chemotaxis model. In the numerical simulations, only two dimensional problems in rectangular domain were considered. Moreover, in his method, the density dependent cross diffusion term is put in the equilibrium distribution function, this procedure is unreasonable from the Chapman–Enskog analysis. In addition, the parallel characteristic of LBM is destroyed since the gradient operator included in the equilibrium distribution function is computed by the finite difference scheme.

In this work, our main aim is to develop an efficient and stable LBM for the generalized K–S chemotaxis model in handling both 2D and 3D problems with arbitrary geometries. In the process of model construction, one of the most critical is that how to process the density dependent cross diffusion term. From the Chapman–Enskog analysis, we found that the cross diffusion term should be put in the evolution equation as a source term rather than in the equilibrium distribution equation. The similar handling way can also be found in our previous work for the Nernst–Planck equation in Ref. [35]. Furthermore, to better capture the singular solutions, a correction term [37] is introduced in the evolution equation to make the proposed LBM more stable. If not, the cell densities may become negative, which will trigger numerical instabilities. In addition, a local scheme for the gradient operator in the correction term is developed, which makes the whole collision process of the proposed coupled LBM be implemented locally. Thus, the coupled LBM can easily handle both 2D and 3D problems with arbitrary geometries. In fact, this proposed model can also be applied to n dimensional problems.

The article is organized as follows. In Section 2, the coupled LBM for the generalized K–S model is proposed. In Section 3, after the validation and discussion of the numerical method, the numerical experiments on several problems are carried out, including the blow up problem in square and circle domains, two-species chemotaxis blow up problems, chemotactic bacteria pattern formation in semi-solid medium in circle domain, 3D pattern formation in liquid medium. Furthermore, the proposed LBM is also extended to the haptotaxis system to simulate tumor invasion into surrounding healthy tissue. At last, some conclusions are summarized in Section 4.

2. The coupled lattice Boltzmann method

In this section, we present the coupled LBM for the generalized K–S model. The evolution equations of the LBM for Eqs. (1a) and (1b) are given by

$$f_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = f_i(\mathbf{x}, t) - \frac{1}{\tau_b}(f_i(\mathbf{x}, t) - f_i^{\mathrm{eq}}(\mathbf{x}, t)) + \Delta t S_i(\mathbf{x}, t) + \Delta t F_i(\mathbf{x}, t) + \frac{\Delta t^2}{2}\partial_t F_i(\mathbf{x}, t), \tag{2a}$$

$$g_i(\mathbf{x}+\mathbf{c}_i\Delta t, t+\Delta t) = g_i(\mathbf{x}, t) - \frac{1}{\tau_s}(g_i(\mathbf{x}, t) - g_i^{\mathrm{eq}}(\mathbf{x}, t)) + \Delta t \bar{S}_i(\mathbf{x}, t) + \Delta t \bar{F}_i(\mathbf{x}, t) + \frac{\Delta t^2}{2}\partial_t \bar{F}_i(\mathbf{x}, t), \tag{2b}$$

where τ_b and τ_s are the dimensionless relaxation factors, $f_i(\mathbf{x}, t)$ and $g_i(\mathbf{x}, t)$ are the distribution functions of particle moving with velocity $\mathbf{c}_i$ at position $\mathbf{x}$ and time t. $S_i(\mathbf{x}, t)$ is defined as

$$S_i(\mathbf{x}, t) = \omega_i\left(\mathbf{c}_i \cdot \beta b(\mathbf{x}, t)\nabla s(\mathbf{x}, t) + \frac{A\mathbf{c}_i \cdot \nabla b(\mathbf{x}, t)}{\tau_b}\right), \tag{3}$$

where the first term on the right hand side of above equation is to deal with the density dependent cross diffusion term and the second term is the correction term to modify $\mu(b, s)$ in Eq. (1a). The weight coefficients ω_i are related to the discrete