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Monte Carlo simulation for kinetic chemotaxis model: An application to the traveling population wave

Shugo Yasuda [1]

Graduate School of Simulation Studies, University of Hyogo, Japan
WPI Immunology Frontier Research Center, Osaka University, Japan

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ABSTRACT

A Monte Carlo simulation of chemotactic bacteria is developed on the basis of the kinetic model and is applied to a one-dimensional traveling population wave in a microchannel. In this simulation, the Monte Carlo method, which calculates the run-and-tumble motions of bacteria, is coupled with a finite volume method to calculate the macroscopic transport of the chemical cues in the environment. The simulation method can successfully reproduce the traveling population wave of bacteria that was observed experimentally and reveal the microscopic dynamics of bacterium coupled with the macroscopic transports of the chemical cues and bacteria population density. The results obtained by the Monte Carlo method are also compared with the asymptotic solution derived from the kinetic chemotaxis equation in the continuum limit, where the Knudsen number, which is defined by the ratio of the mean free path of bacterium to the characteristic length of the system, vanishes. The validity of the Monte Carlo method in the asymptotic behaviors for small Knudsen numbers is numerically verified.

1. Introduction

Due to innovative developments in biotechnology, including tissue engineering and cell engineering, studies on active fluids composed of biological entities have recently drawn increasing attention from physical and mathematical scientists. The pattern formations and fluid flows that are spontaneously generated by the internal motions of active entities, which interact with the local environment, are studied from a physical point of view at both the microscopic and macroscopic levels. A suspension of chemotactic bacteria, e.g., *E. Coli*, is a typical example of the active fluid, in which the bacteria create the collective motions, and the macroscopic patterns are created spontaneously via interactions with chemical cues, whose local concentrations also vary [1–4].

The macroscopic transport phenomena created by the collective motion of chemotactic bacteria can be modeled using the coupled reaction–diffusion equations for nutrients (which are consumed by bacteria), chemoattractants (which are secreted by bacteria), and bacterial density. The basic idea of utilizing the reaction–diffusion equation to describe the collective motion of chemotactic bacteria was first introduced by Keller and Segel [5,6], and both mathematical and physical studies on the Keller–Segel model have accumulated. Although the microscopic basis of the Keller–Segel model was more recently laid by the asymptotic analysis of the kinetic chemotaxis model [7], this type of modeling is originally based on a phenomenological point of view. The macroscopic transport phenomena are consequences of the migrations of bacteria,

E-mail address: yasuda@sim.u-hyogo.ac.jp.
[1] Fax: +81(0)783031990.

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molecular diffusion of chemical cues (i.e., nutrients and chemoattractants), and their mutual interactions [8–11]. Thus, the transport phenomena of chemotactic bacteria set an important multiscale problem to be resolved from physical and mathematical points of view. The mesoscopic model to describe the connection between the microscopic dynamics of bacterium and the macroscopic transports of chemical cues and bacteria population density takes on major significance.

The kinetic approach to describing the collective motion of chemotactic bacteria was first introduced by Alt [12] and then further developed [13]. In the collective motions of the bacteria, each bacterium repeats a simple run-and-tumble motion, where they run ballistically in some duration and subsequently change their directions randomly. In kinetic modeling, the run-and-tumble motion of bacterium is assumed to be a stochastic process, and the time evolution of the density of bacteria with a velocity of $\boldsymbol{v}$, $f(t, \boldsymbol{x}, \boldsymbol{v})$ is described by a variant of the Boltzmann transport equation for gases (although the present kinetic transport equation does not involve the quadratic operator for collisions) [14,15]. The transition (or scattering) kernel in the kinetic chemotaxis equation involves a model response function that stochastically determines the run durations of each bacterium according to the environment experienced by the bacteria along their pathways. The response function takes a major role to reproduce the chemotactic motions of each bacterium and their collective behaviors. Thus, the kinetic approach is a promising candidate to investigate the connection between the microscopic dynamics of bacteria and macroscopic transport phenomena.

Recently, the studies on the kinetic chemotaxis have been actively performed by mathematical scientists. Several researchers have succeeded in deriving the macroscopic continuum equations for chemotactic bacteria from the kinetic transport equation, and the connection between the macroscopic continuum description and the mesoscopic kinetic description has gradually been revealed [16–26]. A comprehensive mathematical study on the traveling wave of the kinetic chemotaxis model is also given by Calvez [27]. The kinetic chemotaxis model has also been utilized in the analysis of the experimental results. Saragosti et al. described the largely biased motions of bacteria toward regions with a high concentration of chemical cues, and they proposed a kinetic model based on experimental observations [28].

The numerical simulations of the kinetic chemotaxis model also takes on a significance in understanding the multiscale mechanism in the collective motions of chemotactic bacteria or analyzing the problems occurring in practical engineering and biological systems. In the simulation methodologies for solving the kinetic chemotaxis models, the difficulty arises in the treatment of the response function in the scattering kernel. It should be noted that the response function depends not only on the instantaneous spatial distribution of chemical cues but on the temporal variations along the running directions of each bacterium. Recently, a Cartesian- mesh-based numerical method to accurately solve the kinetic chemotaxis equation was developed by Yang and Filbet and applied to various one- and two-dimensional problems [29]. In the method, an elaborate numerical algorithm is employed to treat the scattering kernel of the kinetic transport equation.

In the present study, a Monte Carlo simulation method for chemotactic bacteria in a three-dimensional system is newly developed on the basis of the kinetic chemotaxis equation used in Ref. [28], and the Monte Carlo method is applied to the traveling population wave in a microchannel [30–33]. Because the Monte Carlo simulation employs a particle-based method, the treatment of the response function, which may depend on the memory of bacterium along its pathway [30,37–40,42], is simplified. Some numerical studies toward this direction were also put forward by Rousset and Samaey [43,44]. The microscopic dynamics of bacterium and its relation to the macroscopic transports of chemical cues are investigated in detail. The simulation results are also compared to the asymptotic solution obtained from the kinetic chemotaxis model in order to validate the accuracy of the Monte Carlo method in the asymptotic behaviors. Thus, the purpose of the present study is to propose a new Monte Carlo simulation method and to demonstrate the validity and utility of the method numerically. Incidentally, other Monte Carlo simulations, e.g., the Brownian dynamics simulations [34,35] and the velocity-jump simulation involving a memory kernel [36], for the kinetic chemotaxis are also proposed. In the present Monte Carlo method, the velocity jump process described by the kinetic chemotaxis equation involving a response function of the tumbling rate and a persistence of the reorientation angle is utilized.

In Sec. 2, the basic model, i.e., the kinetic chemotaxis model, and its non-dimensional form are described. In Sec. 3, the methodology of the present Monte Carlo simulation is explained in detail. In Sec. 4, the numerical results of the Monte Carlo simulations are presented for the macroscopic transports, the microscopic dynamics, and the effects of variations in the parameters of the response function. Special focus is placed on the relation between the microscopic dynamics of bacterium and the macroscopic transports of the chemical cues and bacteria population density. In Sec. 5, the results of Monte Carlo simulations are compared to the asymptotic solution of the kinetic chemotaxis model in the continuum limit to examine the accuracy of the Monte Carlo method in the asymptotic behaviors. Finally, concluding remarks and an outlook are given in Sec. 6.

2. Basic model

The basic model is described in the reference [28]. In the modeling, the macroscopic transport of chemical cues, i.e., the nutrients consumed by bacteria and the chemoattractants secreted by bacteria, is described by continuum reaction–diffusion equations, whereas the run-and-tumble motions of bacteria are described by a kinetic equation. Because a small bacterium, e.g., *E. coli*, is assumed, the cells are not able to choose directly the preferential direction of motion toward the region of a high concentration of chemical cues by measuring the head-to-tail gradient of the chemical cues. Instead, the cells detect the preferential direction by sensing the temporal variation of chemical cues experienced along their pathways. This sensing strategy of bacteria is accounted for in the response function in the kinetic equation.

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