Lattice Boltzmann simulation for the spiral waves in the excitable medium

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Abstract: We propose lattice Boltzmann method for the spiral waves. Using Chapman-Enskog expansion and multiscales technique, we obtain equilibrium distribution functions of the model. As an example, we simulate the Selkov reactions with scratching mark, i. e. using a scratching mark pacemaker, obtained one classical spiral waves.

Keywords: lattice Boltzmann method, excitable medium, Selkov system, spiral waves

Introduction

Much research in the nonequilibrium physics of excitable media has been motivated by the observation of dynamical states containing defects, i. e., spiral waves in two space dimension or spiral filaments in three dimensions[1]. The spiral waves is the chemical system of ordered structures decided by the nonlinear feature far from the states of equilibrium. Its density changes by the time on the spatial distributions. By experimental studies, many types of waves have been found, such as target waves, spiral waves, mosaic structure, crescent shape, etc.[2] But, for a long time, there has been two difficulties in numerical simulation of chemical waves: (1) We do not understand well the excitable media in mathematical concepts. Now, a simple, linear and local expression is that the Jacobean possess an eigenvalue with navigate real part. (2) There are no defects in diffusion-reaction equations. Many studies show that the defect is the condition on the appearance of spiral waves. Therefore, scientists plan have offered many methods to describe the defect, for example, Barkley method[3], scratching mark pacemaker, and adding gravity by slopping the vessels[4]. These methods are effective but complex for numerical simulation. In this letter, we propose a simple lattice Boltzmann method for the spiral waves by adjusting the equilibrium distribution functions of the model, obtained the Selkov system[5],

$$A \rightleftharpoons X, \quad X + 2Y \rightleftharpoons 3Y, \quad Y \rightleftharpoons B$$

We simulate the nonlinear reactions in the Selkov system, then using scratching mark pacemaker, obtain the spiral waves in the excitable media.

The Celluar Automata is an available method for the spiral waves[6,7], but this method is confined by the computer memory[8]. Fortunately, an artificial system, lattice Boltzmann model may be constructed which is simple enough to be used on the computer, but yet contain all the required physics of a realistic fluid system[8-11]. Now, many researchers have focus on the lattice Boltzmann model for chemical reactions[12,13].

Lattice Boltzmann method has been adopted as an alternative numerical scheme for simulation of fluid flows, which comes from the Cellular Automaton and BGK type Boltzmann equations. This method possesses simple codes, higher order of truncation error and higher resolutions for the Navier-Stokes equations[14-16]. Specially, for two-dimension and three-dimension flows, the scheme is the same as the one-dimensional coordinate. If the chemical system has not convection effects, the lattice Boltzmann model will be simpler than other models.

1 Lattice Boltzmann model

Let us define $f_\alpha^\sigma(x,t)$ as the one-particle distribution function of species σ, with velocity e_α at time t, and position x. The coordinate x only takes on a discrete set of values: the nodes of the chosen lattice. All the simulations that we show in the paper have been done in two spatial dimensions using a square lattice of unit size. The nearest neighbor vectors are defined as

$$e_\alpha = i\cos\frac{(\alpha-1)\pi}{2} + j\sin\frac{(\alpha-1)\pi}{2}, \quad 1 \le \alpha \le 4$$

where i and j are unit vectors alone the x and y directions, respectively. In addition, we use the particle at rest: $e_\alpha = 0$. Thus at each lattice site, we have five states for each species. The macroscopic quantity is defined by

$$u^\sigma = \sum_\alpha f_\alpha^\sigma(x,t)$$

where $\sigma = 1,2,\cdots,M$ and M is species numbers. The lattice Boltzmann equations can be written as

$$f_\alpha^\sigma(x+\Delta x,t+\Delta t) - f_\alpha^\sigma(x,t) = -\frac{1}{\tau}[f_\alpha^\sigma(x,t) - f_\alpha^{\tau,\text{eq}}(x,t)] + \omega_\alpha^\sigma(x,t) \tag{1}$$

where $f_\alpha^{\sigma,\text{eq}}(x,t)$ is the local equilibrium distribution function, ω_α^σ is the additional term, and τ is the single relaxation factor.

According to Refs. [15, 16], we obtain the local equilibrium distribution functions

$$f_0^{\sigma,\text{eq}} = u^\sigma - \frac{\lambda^\sigma du^\sigma}{c^2}, \quad f_\alpha^{\sigma,\text{eq}} = \frac{\lambda^\sigma du^\sigma}{bc^2}, \quad \alpha = 1,\cdots,b$$

where $c = |e_\alpha|$, $d = 2$ is the spatial dimensional numbers, $\lambda^\tau = D^\sigma/\varepsilon(\tau - 0.5)$, and D^σ the diffusion coefficients. We also get the diffusion reaction Eq. (2) when using the hypothesis $\omega_\alpha^\sigma = \varepsilon^2\varphi_\alpha^\sigma$:

$$\frac{\partial u^\sigma}{\partial t} = D^\sigma\nabla^2 u^\sigma + (b+1)\varepsilon\phi^\sigma(u^\sigma) + O(\varepsilon^2) \tag{2}$$

By simple selection: $\rho_1 = u^1$, $\rho_2 = u^2$, we have the Selkov reaction system as follows[5,12]:

$$\frac{\partial\rho_1}{\partial t} = D_1\nabla^2\rho_1 + k_1\rho_a - k_{-1}\rho_1 - k_2\rho_1\rho_2^2 + k_{-2}\rho_2^3 \tag{3}$$

$$\frac{\partial\rho_2}{\partial t} = D_2\nabla^2\rho_2 + k_{-3}\rho_b - k_3\rho_2 + k_2\rho_1\rho_2^2 - k_{-2}\rho_2^3 \tag{4}$$

where ρ_a, ρ_b, k_i and k_{-i} are the system parameters, D_1 and D_2 are diffusion coefficients.

2 Numerical simulation

Combining Eqs. (3) and (4), we set

$$(b+1)\varepsilon\phi^1(u^1) = k_1\rho_a - k_{-1}\rho_1 - k_2\rho_1\rho_2^2 + k_{-2}\rho_2^3$$

$$(b+1)\varepsilon\phi^2(u^2) = k_{-3}\rho_b - k_3\rho_2 + k_2\rho_1\rho_2^2 - k_{-2}\rho_2^3$$

and

$$\lambda^1 = \frac{D_1}{\varepsilon(\tau - 0.5)}, \quad \lambda^2 = \frac{D_2}{\varepsilon(\tau - 0.5)}$$

thus, we can iterate Eq. (1) from time step t to $t + \Delta t$. Now, we express the densities ρ_1, ρ_2 in multi-scale

$$\rho_\sigma = \varepsilon \rho_\sigma^{(0)} + \varepsilon^2 \rho_\sigma^{(1)} + \varepsilon^3 \rho_\sigma^{(2)} + O(\varepsilon^4)$$

where $\rho_\sigma^{(0)}$ is the local stable resting point, $\sigma = 1, 2$. Thus,

$$\rho_\sigma^{(1)} = \frac{\left(\rho_\sigma - \varepsilon \rho_\sigma^{(0)}\right)}{\varepsilon^2}, \quad \rho_\sigma^{(2)} = \frac{\left(\rho_\sigma - \varepsilon \rho_\sigma^{(0)} - \varepsilon^2 \rho_\sigma^{(1)}\right)}{\varepsilon^3}$$

As numerical example, we select scratching mark pacemaker method for initial values, and using the periodic boundary conditions in the x direction, and the $\nabla \rho_\sigma = 0$ boundary condition in the y direction. Fig. 1 shows spiral waves of the $\rho_\sigma^{(1)}$ ($\sigma = 1, 2$) fields in scale ε^2 at time $T = 2000\Delta t$. The lattice size is 100×100, diffusion coefficients are $D_1 = 3/4$ and $D_2 = D_1/16$.

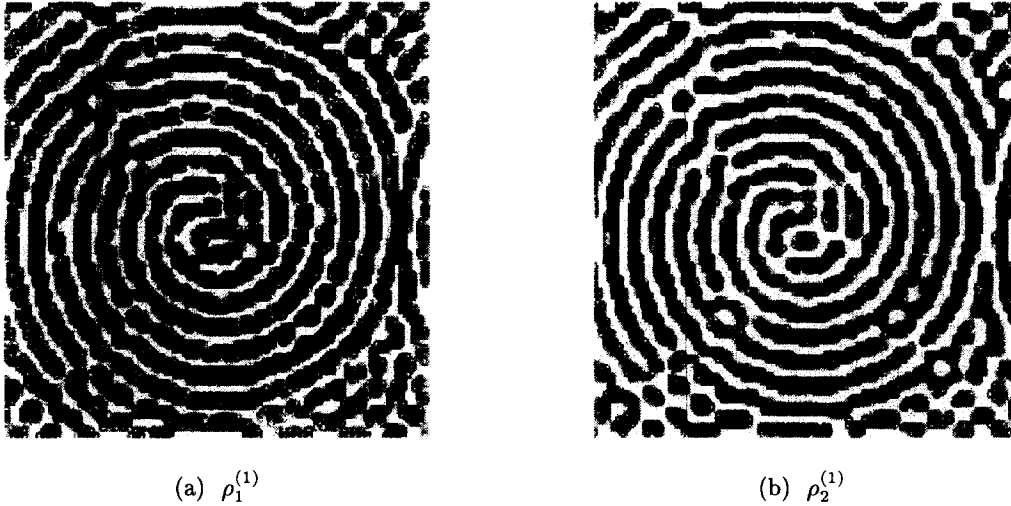(a) $\rho_1^{(1)}$ (b) $\rho_2^{(1)}$

Fig. 1 Spiral waves formation in the Selkov reaction by fields of $\rho_1^{(1)}$ and $\rho_2^{(1)}$. Parameters: $c = 10$, $\varepsilon = 0.05$, $\tau = 1/1.3$, $b = 4$, $D = 2$, $\Delta x = 0.5$, $\Delta t = 0.05$, $k_1 \rho_a = 1.07273$, $k_3 = 10/22$, $k_{-1} = 1/22$, $k_{-3}\rho_b = 0.109091$, $k_2 = k_{-2} = 1/20$, $T = 2000\Delta t$. Lattice size 100 × 100. Gray levels: 100

A spiral wave can be generated from a ring of excitation by shearing the ring to produce free ends which can form the cores of two counter rotating spiral waves[17]. This is a feature of excitable media, which can be generated from a spontaneous nucleation. This spontaneous nucleation can be set as a source of the pacemaker[18]. Nevertheless, if the medium is excitable enough, the numerical simulation may be successful, while if the excitable is too weak, the spontaneous nucleation may be diluted. The method of scratching mark pacemaker can keep non-symmetry till the spiral waves appear.

3 Conclusions

In this paper, we presented a lattice Boltzmann scheme for the numerical simulation of the spiral waves. We obtained a classical result of chemical waves. It is difficult to keep convection effect in experiments, but in the scheme, we give a simple equilibrium distribution function, which can yield non-convection effect easily. We also used the assumption $\omega_\alpha^\sigma = \varepsilon^2 \varphi_\alpha^\sigma$, which is very important in constructing the model[15]. As a preliminary conclusion, we consider the

spiral wave possesses multiscale structures. The spiral structure is in scale ε^2. The next work may be to explore new chemical waves and Turing patterns in other scales or research into the relationship between spiral movement and other physical factors.

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