Recovery of the scale-ε^2 pattern by lattice BGK model

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Abstract: A lattice BGK method for nonlinear chemical reactions is described. Since the equation does not possess the convect terms, we can easily get the equilibrium distribution functions of the lattice BGK models. Using this model, we consider the scales- ε^2 patterns, find two types of pattern: mosaic structure and the Turing pattern.

Keywords: lattice BGK method, Turing pattern, mosaic structure

Introduction

The chemical oscillation and chemical waves are the chemical system of the order structures decided by the nonlinear features far from the state of equilibrium. If we consider the effect of the diffusion and nonlinear reaction, then we can find two types of chemical phenomena: Turing pattern and nonlinear chemical waves[1-3]. Turing pattern is the periodic structure in the spatial distribution. In 1952, Turing pointed out that the structure exists. The character of the Turing pattern is that the stable spatial structure is distorted from the state of equilibrium. It relies on some parameters, such as diffusion coefficient, the densities of the species, reaction speeds, *etc.* Nevertheless, it is difficult to produce the Turing patterns by experiments. There are three reasons for the difficulty: (1) we cannot control the reaction conditions, (2) we can not remove the convect effect, (3) we cannot find the multiscale of the Turing pattern.

We have much interest on the Turing patterns and dynamical behavior that can be used to study and comprehend the complicate phenomena. In this paper, we focus on the following problems: (1) a lattice BGK model for the nonlinear chemical reaction, (2) the behavior of the Turing patterns, (3) the resolution of sharp gradient region.

It is known that self-organization phenomena are statistical behaviors of their associated microscopic system. This system seems to be thermodynamically described by the Boltzmann equation. Fortunately, due to the non-unique correspondence between a self-organization system and microscopic system, an artificial system we called "mesoscopic system", may be constructed which is simple enough to be simulate on a computer. According to this idea, a computational approach called lattice BGK method has recently been developed[4-7]. The main idea of lattice BGK model is to get available macroscopic physical equations by using the BGK type Boltzmann equation. In general, time, space and velocity are discrete on one lattice, and then choose the equilibrium distribution function to fit some requirements which can be obtained with multiscale technique and Chapman-Enskog expansion[8-10].

1 Lattice BGK model

In this lattice BGK model, we discrete the velocity of the particles into b directions. The lattice with unit spacing is used which each node has b nearest neighbors connected with b links.

These particles' velocities are e_α. The macroscopic quality u is defined by

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

where f_α is the single-particle distribution function at time t, node x with velocity e_α. The lattice Boltzmann equation may read[8,9,11]

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

where $f_\alpha^{\text{eq}}(x, t)$ is the local equilibrium distribution function at time t, node x, with velocity e_α, τ is the single relaxation time factor, and ω is the additional term.

We select a small parameter ε as the time unit in numerical simulation, it also can play the role of the Knudsen number[10]. By using multi-scale method and Chapman-Enskog expansion, we get a series of lattice Boltzmann equations on different time scales and a conservation law on the first time scale t_0 [9,10]. It is suitable to use an assumption $\omega = \varepsilon^2 \phi(u)$, thus we obtain

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

where $\lambda = D/\varepsilon(\tau - 0.5)$, $c = |e_\alpha|$, d is the dimensional number, D the diffusion coefficients. In conclusion, the macroscopic equation is

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

2 Numerical simulation

2.1 The Schlogl model and its mosaic structure

According to Eq. (1), we select

$$(b+1)\varepsilon\phi(u) = -k(u^3 - 1.5u^2 + 0.6875u - 0.09375)$$

where $k = 0.01$ [11]. This equation is the Schlogl model with bistable regions[11-13]. By simple algebra, the higher density $u_H = 0.75$, and lower density $u_L = 0.25$. Now, we express the density u as multi-scale expansion

$$u = u_0 + \varepsilon u_1 + \varepsilon^2 u_2 + O(\varepsilon^3)$$

where u_0 is the solution of the equation $\phi(u) = 0$. Thus,

$$u_1 = \frac{u - u_0}{\varepsilon}, \quad u_2 = \frac{u - u_0 - \varepsilon u_1}{\varepsilon^2}$$

In this paper, we simulate a two-dimensional reaction using lattice BGK method. By selecting two diffusion coefficients, we find the width of sharp gradient (resolution) relies on D. We plot the numerical simulation results (Fig. 1). The lattice size is 50×50 with random initial conditions and $\nabla u = 0$ boundary conditions. The diffusion coefficient is $D = 1.0 \times 10^{-3}$. We find these Turing patterns have three regions, higher density, u_H (gray), lower density, u_L (black), and sharp gradient (bright) (see Fig. 1a). In this situation, the diffusive effect offsets generated effect, the lower density region exists when $T > 1500\Delta t$. We also examine the case $T > 10^6\Delta t$, find the lower density region still exists. In Fig. 1b, we give the Turing patterns of u_1. It shows a mosaic structure. The physical meaning is that two u_0's generate two u_1's.

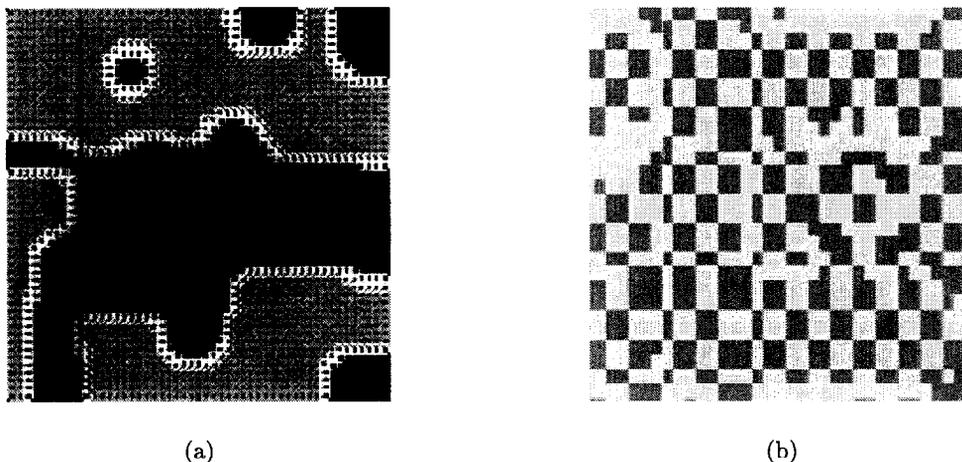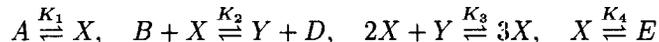(a)   (b)

Fig. 1   (a)   Turing pattern of the Schlogl model at time step $T = 10000\Delta t$, higher density (gray) $u_H = 0.75$, lower density (black) $u_L = 0.25$, and region of sharp gradient (bright). Lattice size is 50×50. Parameters: $\tau = 1/1.2$, $c = 3.0$, $b = 4$, $d = 2$, $D = 1.0 \times 10^{-3}$, $\Delta x = 0.02$, $\Delta t = \Delta x/c$. (b)   A mosaic structure in the Schlogl reaction within the black region (see (a)) at time step $T = 10000\Delta t$. Parameters the same as (a)

2.2   The Belousov-Zhabotinskii reaction

The Belousov-Zhabotinskii reaction has six species, four steps reactions[12],

$$A \overset{K_1}{\rightleftharpoons} X, \quad B + X \overset{K_2}{\rightleftharpoons} Y + D, \quad 2X + Y \overset{K_3}{\rightleftharpoons} 3X, \quad X \overset{K_4}{\rightleftharpoons} E$$

The reaction equations are

$$\frac{\partial u}{\partial t} = \xi - (\eta + 1)u + u^2 v + D_1 \nabla^2 u$$

$$\frac{\partial v}{\partial t} = \eta u - u^2 v + D_2 \nabla^2 v$$

In this paper, we select the parameters as $\xi = 2.0$, $\eta = 5.45$ for the reaction terms. The diffusion coefficients are $D_1 = 8.0 \times 10^{-3}$, $D_2 = 4.0 \times 10^{-3}$. Parameters in the lattice Boltzmann equation: $c = 3.0$, $1/\tau = 1.2$, $b = 4$. For this test, we use two layers lattice to simulate. These additional terms in layers lattice u and v are given as follows:

$$\phi^u = \frac{1}{\varepsilon(b+1)}[\xi - (\eta + 1)u + u^2 v], \quad \phi^v = \frac{1}{\varepsilon(b+1)}[\eta v - u^2 v]$$

with boundary conditions $\nabla u = \nabla v = 0$ and random initial values.

In Fig. 2, we give two-dimensional numerical simulation result by using lattice BGK method. The lattice size is 100×100 with random initial condition and $\nabla u = \nabla v = 0$ boundary conditions. It shows that results have multi-scale structures. In Fig. 2a, we plot the density gray picture in the scale ε, which appears a target wave. The reason is that the diffusion effect is greater than the reaction effect. In Fig. 2b and 2c, we give two ε^2 scale gray pictures, i. e., pattern of u_1. Fig. 2b (40 gray-levels), Fig. 2c (300 gray-levels) show periodic spatial structures. According to the definition of the Turing pattern, Fig. 2b and 2c are Turing patterns with periodic structures.

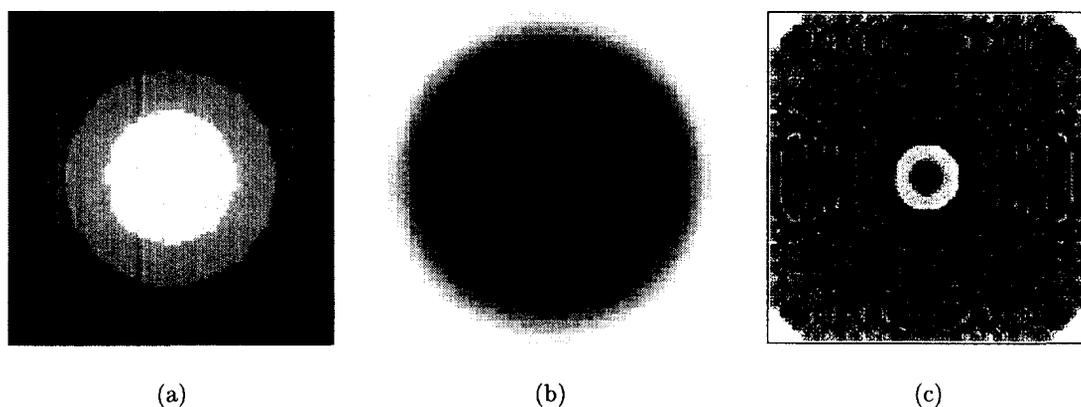(a)   (b)   (c)

Fig. 2 (a) Target wave in the Belousov-Zhabotinskii reaction at time steps $T = 2000\Delta t$. Parameters for the reaction terms: $A = 2.0$, $B = 5.45$ and $L = 1.0$. The diffusion coefficients: $D_1 = 8.0 \times 10^{-3}$, $D_2 = 4.0 \times 10^{-3}$. Parameters in the lattice Boltzmann equation: $c = 3.0$, $1/\tau = 1.2$, $b = 4$, $d = 2$, $\Delta x = 0.01$, $\Delta t = \Delta x/c$, gray levels = 8. (b), (c) Turing patterns of the Belousov-Zhabotinskii reaction in scale ε^2 at time steps $T = 2000\Delta t$. Parameters the same as (a) but (b) with gray-levels = 40, (c) with gray-levels = 300

2.3 The resolution of sharp gradient

We are interested in the resolution of sharp gradient. Let $S(x)$ is the Boolean variable, $S(x) = 1$, if $|\nabla u| > (|\nabla u|_{max} + |\nabla u|_{min})/2$; $S(x) = 0$, otherwise. Then Hamming length $H = \sum\limits_{i=1}^{M} S(x_i)$ is the cell number of the resolution on sharp gradient, where i is the footnote of lattice note x_i. Our result is 3–5 cells (see Fig. 3). We find the resolution relies on the diffusion coefficient. This idea can be used to examine other problems, e. g., shock wave and contact interface.

3 Conclusions

In this paper, we present a lattice BGK model for nonlinear chemical reactions, and get the mosaic structure and spatial periodic structure. We also give a method to find the resolution of sharp gradient regions. An important result is that the Turing patterns appear in scale-ε^2. These numerical results may be new things. In summary, the nonlinear chemical waves possess multi-scale structures, which have different patterns.
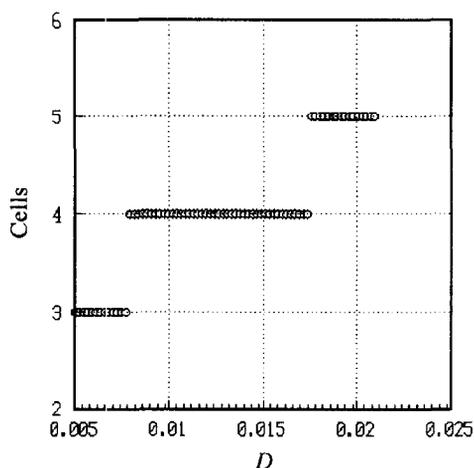

Fig. 3 Scatter graphics of the cell numbers (resolution) about the sharp gradient vs diffusion coefficient D, at line $y = 0.5$. Parameters the same as Fig. 1a

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