Lattice Boltzmann Simulation of Some Nonlinear Complex Equations

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Abstract. In this paper, the lattice Boltzmann method for convection-diffusion equation with source term is applied directly to solve some important nonlinear complex equations, including nonlinear Schrödinger (NLS) equation, coupled NLS equations, Klein-Gordon equation and coupled Klein-Gordon-Schrödinger equations, by using complex-valued distribution function and relaxation time. Detailed simulations of these equations are carried out. Numerical results agree well with the analytical solutions, which show that the lattice Boltzmann method is an effective numerical solver for complex nonlinear systems.

Keywords: Lattice Boltzmann method, nonlinear Schrödinger equation, Klein-Gordon equation, Klein-Gordon-Schrödinger equations.

1 Introduction

The lattice Boltzmann method (LBM) is an innovative computational fluid dynamics (CFD) approach for simulating fluid flows and modeling complex physics in fluids [1]. Compared with the conventional CFD approach, the LBM is easy for programming, intrinsically parallel, and it is also easy to incorporate complicated boundary conditions such as those in porous media. The LBM also shows potentials to simulate the nonlinear systems, including reaction-diffusion equation [2,3,4], convection-diffusion equation [5,6], Burgers equation [7] and wave equation [3,8], etc. Recently, a generic LB model for advection and anisotropic dispersion equation was proposed [9]. However, almost all of the existing LB models are used for real nonlinear systems. Beginning in the mid 1990s, based on quantum-computing ideas, several types of quantum lattice gases have been studied to model some real/complex mathematical-physical equations, such as Dirac equation, Schrödinger equation, Burgers equation and KdV equation [10,11,12,13,14,15,16,17]. Although these work are not in the classical LBM framework, they bring us an interesting problem: how does the classical LBM work when used to model complex equations? Very recently, Linhao Zhong, Shide Feng, Ping Dong, et al. [18] applied the LBM to solve one-dimensional nonlinear Schrödinger (NLS) equation using the idea of quantum lattice-gas model [13,14] for treating the reaction term. Detailed simulation results in Ref.[18] have shown that the LB schemes proposed have accuracy that is better than or at least comparable to the Crank-Nicolson finite difference scheme. Therefore, it is necessary to study the LBM for nonlinear complex equations further.

In this paper, using the idea of adopting complex-valued distribution function and relaxation time [18], the LBM for n -dimensional (n D) convection-diffusion equation (CDE) with source term is applied directly to solve some important nonlinear complex equations, including nonlinear Schrödinger (NLS) equation, coupled NLS equations, Klein-Gordon (KG) equation and coupled Klein-Gordon-Schrödinger (CKGS) equations. Detailed simulations of these equations are carried out for accuracy test. Numerical results agree well with the analytical solutions, which show that the LBM is also an effective numerical solver for complex nonlinear systems.

2 Lattice Boltzmann Model

The n D CDE with source term considered in this paper can be written as

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \alpha \nabla^2 \phi + F(\mathbf{x}, t), \quad (1)$$

where ∇ is the gradient operator with respect to the spatial coordinate $\mathbf{x}$ in n dimensions. ϕ is a scalar function of time t and position $\mathbf{x}$. $\mathbf{u}$ is a constant velocity vector. $F(\mathbf{x}, t)$ is the source term. When $\mathbf{u} = 0$, Eq.(1) becomes the diffusion equation (DE) with source term, and several of such equations form a reaction-diffusion system (RDS).

2.1 LB Model for CDE

The LB model for Eq.(1) is based on the $DnQb$ lattice [1] with b velocity directions in n D space.

The evolution equation of the distribution function in the model reads

$$f_j(\mathbf{x} + \mathbf{c}_j \Delta t, t + \Delta t) - f_j(\mathbf{x}, t) = -\frac{1}{\tau} (f_j(\mathbf{x}, t) - f_j^{eq}(\mathbf{x}, t)) + \Delta t F_j(\mathbf{x}, t), \quad j = 0, \dots, b-1, \quad (2)$$

where $\{\mathbf{c}_j, j = 0, \dots, b-1\}$ is the set of discrete velocity directions, Δx and Δt are the lattice spacing and the time step, respectively, $c = \Delta x / \Delta t$ is the particle speed, τ is the dimensionless relaxation time, and $f_i^{eq}(\mathbf{x}, t)$ is the equilibrium distribution function which is determined by

$$f_j^{eq}(\mathbf{x}, t) = \omega_j \phi \left(1 + \frac{\mathbf{c}_j \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{u}\mathbf{u}) : (\mathbf{c}_j \mathbf{c}_j - c_s^2 \mathbf{I})}{2c_s^4} \right) \quad (3)$$

such that

$$\sum_j f_j = \sum_j f_j^{eq} = \phi, \quad \sum_j \mathbf{c}_j f_j^{eq} = \phi \mathbf{u}, \quad \sum_j \mathbf{c}_j \mathbf{c}_j f_j^{eq} = c_s^2 \phi \mathbf{I} + \phi \mathbf{u} \mathbf{u} \quad (4)$$

with $\alpha = c_s^2 (\tau - \frac{1}{2}) \Delta t$, where $\mathbf{I}$ is the unit tensor, ω_j are weights and c_s , so called sound speed in the LBM for fluids, is related to c and ω_j . They depend on the lattice model used.

For the D1Q3 model, $\omega_0 = 2/3$, $\omega_{1 \sim 2} = 1/6$, for the D2Q9 one, $\omega_0 = 4/9$, $\omega_{1 \sim 4} = 1/9$, $\omega_{5 \sim 8} = 1/36$, then $c_s^2 = c^2/3$ for both of them.

F_j in Eq.(2), corresponding to the source term in Eq.(1), is taken as

$$F_j = \omega_j F \left(1 + \lambda \frac{\mathbf{c}_j \cdot \mathbf{u}}{c_s^2} \right) \quad (5)$$

such that $\sum_j F_j = F$, $\sum_j \mathbf{c}_j F_j = \lambda F \mathbf{u}$, where λ is a parameter which is set to be $\frac{\tau - \frac{1}{2}}{\tau}$ in the paper. It is found that the LB model using this setting has better numerical accuracy and stability when $\mathbf{u} \neq \mathbf{0}$.

The macroscopic equation (1) can be derived though the Chapman-Enskog expansion (See Appendix for details). It should be noted that the equilibrium distribution function for above LBM was often used in linear form of $\mathbf{u}$, which is different from that in Eq.(3). However, from the appendix we can see that some additional terms in the recovered macroscopic equation can be eliminated if Eq.(3) is used. Moreover, if $\mathbf{u}$ is not constant, the appropriate assumption on it is needed in order to remove the additional term(s) when recovering Eq.(1).

2.2 Version of LB Model for Complex CDE

Almost all of the existing LB models simulate the real evolutionary equations. However, from the Chapman-Enskog analysis, we can find that the functions in CDE and related distribution function can be both real and complex without affecting the results. In general, for the complex evolutionary equations, let us decompose the related complex functions and relaxation time into their real and imaginary parts by writing

$$f_j = g_j + \mathbf{i} h_j, f_j^{eq} = g_j^{eq} + \mathbf{i} h_j^{eq}, F_j = G_j + \mathbf{i} H_j, w = \frac{1}{\tau} = w_1 + \mathbf{i} w_2, \quad (6)$$

where $\mathbf{i}^2 = -1$.

Now we can rewrite Eq.(2) as

$$\begin{aligned} & g_j(\mathbf{x} + \mathbf{c}_j \Delta t, t + \Delta t) - g_j(\mathbf{x}, t) = -w_1(g_j(\mathbf{x}, t) - g_j^{eq}(\mathbf{x}, t)) \\ & + w_2(h_j(\mathbf{x}, t) - h_j^{eq}(\mathbf{x}, t)) + \Delta t G_j(\mathbf{x}, t), \\ & h_j(\mathbf{x} + \mathbf{c}_j \Delta t, t + \Delta t) - h_j(\mathbf{x}, t) = -w_2(g_j(\mathbf{x}, t) - g_j^{eq}(\mathbf{x}, t)) \\ & - w_1(h_j(\mathbf{x}, t) - h_j^{eq}(\mathbf{x}, t)) + \Delta t H_j(\mathbf{x}, t), \\ & j = 0, \dots, b-1. \end{aligned} \quad (7)$$

Eq.(7) is the implemental version of the LB model proposed for complex CDE. It should be noted that Eq.(7) reflects the coupling effect of real and imaginary parts of unknown function in complex CDE through the complex-valued relaxation time in a natural way.

3 Simulation Results

To test the LB model proposed above, numerical simulations of some CDEs with source term are carried out. Here we select three types of complex nonlinear evolutionary equations with analysis solutions to test mainly the numerical order of accuracy of the LBM. In simulations, the initial value of distribution function is taken as that of its equilibrium part at time $t = 0$, which is a commonly used

strategy, and $\Delta x^2/\Delta t (= \Delta x \times c)$ is set to be constant for different grids due to some claims that LB schemes are second-order accurate in space and first-order accurate in time.

Example 3.1. We show an accuracy test for the 2D NLS equation

$$\mathbf{i}u_t + u_{xx} + u_{yy} + \beta|u|^2u = 0, \quad (8)$$

which admits a progressive plane wave solution [19]

$$u(x, y, t) = A \exp(\mathbf{i}(c_1x + c_2y - \omega t)), \quad (9)$$

where $\omega = c_1^2 + c_2^2 - \beta|A|^2$; A, c_1 and c_2 are constants.

In simulations, a D2Q9 LB model is used. We set $A = c_1 = c_2 = 1, \beta = 2$ and use the periodic boundary condition is used in $[0, 2\pi] \times [0, 2\pi]$ as in Ref.[19], while the initial condition for u is determined by the analytical solution (9) at $t = 0$. The global relative L^1 error and the numerical order of accuracy are contained in Table 1 at time $t = 1$. From the table we can see that the LBM for the NLS equation (8) has about second-order of accuracy, but the order of accuracy decreases as the resolution increases.

Table 1. Accuracy test for the NLS equation (8)

Grid $N \times N$	c	Real part of u		Imaginary part of u	
		L^1 err	Order	L^1 err	Order
62×62	50	2.56e-2	-	2.57e-2	-
124×124	100	5.71e-3	2.1646	5.71e-3	2.1702
248×248	200	1.34e-3	2.0913	1.34e-3	2.0913
496×496	400	4.15e-4	1.6910	4.15e-4	1.6910

Example 3.2. We show an accuracy test for the 1D coupled NLS equation

$$\begin{aligned} \mathbf{i}u_t + \mathbf{i}\alpha u_x + \frac{1}{2}u_{xx} + (|u|^2 + \beta|v|^2)u &= 0, \\ \mathbf{i}v_t - \mathbf{i}\alpha v_x + \frac{1}{2}v_{xx} + (\beta|u|^2 + |v|^2)v &= 0, \end{aligned} \quad (10)$$

with the soliton solutions [19]

$$\begin{aligned} u(x, t) &= A \operatorname{sech}(\sqrt{2a}(x - \gamma t)) \exp(\mathbf{i}((\gamma - \alpha)x - \omega t)), \\ v(x, t) &= A \operatorname{sech}(\sqrt{2a}(x - \gamma t)) \exp(\mathbf{i}((\gamma + \alpha)x - \omega t)), \end{aligned} \quad (11)$$

where $A = \sqrt{\frac{a}{1+\beta}}, \omega = \frac{\gamma^2 - \alpha^2}{2} - a$; a, γ, α and β are real constants.

We can use two LB evolutionary equations based on D1Q3 lattice to simulate Eq.(10). We set $a = 1, \gamma = 1, \alpha = 0.5, \beta = 2/3$ and use the periodic boundary condition in $[-25, 25]$ as in Ref.[19], while the initial condition is determined by the analytical solution (11) at $t = 0$. The global relative L^1 errors are plotted in Fig. 1 (left) at time $t = 1$ for $\Delta x = 1/10$ to $1/320$, and $c = 20$ to 640 . It is found that the LBM for the coupled NLS equations (10) has the second-order

of accuracy, and the order of accuracy is nearly fixed to 2.0 for different grid resolution. To test the LBM further the error evolution with time is also plotted in Fig.1 (right) for $\Delta x = 1/100$, and $\Delta t = 10^{-4}$ and 10^{-5} , respectively. The errors for $\Delta t = 10^{-4}$ are about 7.0 to 9.0 times those for $\Delta t = 10^{-5}$.

Fig. 1. Left: Global relative errors vs. space steps at $t = 1.0$; Right: Error evolves with time

Example 3.3. Consider the 1D coupled KGS equations

$$\begin{aligned} i\psi_t + \frac{1}{2}\psi_{xx} + \psi\phi &= 0, \\ \phi_{tt} - \phi_{xx} + \phi - |\psi|^2 &= 0, \end{aligned} \quad (12)$$

with the soliton solutions [20]

$$\begin{aligned} \psi(x, t) &= \frac{3\sqrt{2}}{4\sqrt{1-v^2}} \text{sech}^2 \frac{1}{2\sqrt{1-v^2}}(x - vt - x_0) \exp(i(vx + \frac{1-v^2+v^4}{2(1-v^2)}t)), \\ \phi(x, t) &= \frac{3}{4(1-v^2)} \text{sech}^2 \frac{1}{2\sqrt{1-v^2}}(x - vt - x_0), \end{aligned} \quad (13)$$

where v is the propagating velocity of wave and x_0 is the initial phase.

Note that the KG equation in Eq.(12) is different from RD equation, the special case of Eq.(1), due to the second time differential of ϕ . In order to solve this equation by LBM, we must modify the LB model in section 2.

Consider the n D KG equation

$$\phi_{tt} - \alpha \nabla^2 \phi + V(\phi) = 0, \quad (14)$$

in the spacial region Ω , where $V(\phi)$ is some nonlinear function of ϕ . The the initial conditions associated with Eq.(14) are given by

$$\phi(\mathbf{x}, 0) = f(\mathbf{x}), \phi_t(\mathbf{x}, 0) = g(\mathbf{x}), \quad (15)$$

where the boundary conditions can be found according to the given problem.

Using the idea in Ref.[8], we modify Eq.(3) as follows

$$\begin{aligned} f_j^{eq}(\mathbf{x}, t) &= \omega_j \left(\phi_t + \frac{c_s^2(\phi - \phi_t) \mathbf{I} : (\mathbf{C}_j \mathbf{C}_j - c_s^2 \mathbf{I})}{2c_s^4} \right) \\ &= \omega_j \left(\phi_t + \frac{(\phi - \phi_t)(\mathbf{C}_j^2 - nc_s^2)}{2c_s^2} \right), \end{aligned} \quad (16)$$

such that

$$\sum_j f_j = \sum_j f_j^{eq} = \phi_t, \sum_j \mathbf{c}_j f_j^{eq} = \mathbf{0}, \sum_j \mathbf{c}_j \mathbf{c}_j f_j^{eq} = c_s^2 \phi \mathbf{I} \quad (17)$$

with $\alpha = c_s^2(\tau - \frac{1}{2})\Delta t$. We use the difference scheme for computing ϕ_t to obtain ϕ . For instance, $\phi(\mathbf{x}, t + \Delta t) = \Delta t \sum_j f_j(\mathbf{x}, t + \Delta t) + \phi(\mathbf{x}, t)$.

Now we can use two LB evolutionary equations based on D1Q3 lattice to simulate Eq.(12), one for NLS equation and the other for KG equation. In simulation, the initial and boundary conditions are determined by the analytical solution (13) in $[-10, 10]$. The non-equilibrium extrapolation scheme [21] is used for treating the boundary conditions. The global relative L^1 errors are also plotted in Fig. 1 (left) for $v = 0.8, x_0 = 0$ at time $t = 1$ for $\Delta x = 1/10$ to $1/640$, and $c = 10$ to 640 . It is found that the LBM for the coupled KGS equations (12) has also the second-order of accuracy, which is comparable to the multisymplectic scheme in Ref.[20]. We also find that the order of accuracy for ϕ increases from 1.7308 to 2.0033 as the grid resolution increases. This may be because that we use the first-order difference scheme to compute ϕ_t .

4 Conclusion

In this paper the LBM for n D CDE with source term has been applied directly to solve some important nonlinear complex equations by using complex-valued distribution function and relaxation time, and the LB model for n D KG equation is derived by modifying the method for CDE. Simulations of 2D NLS equation, 1D coupled NLS equations and 1D coupled KGS equations are carried out for accuracy test. Numerical results agree well with the analytical solutions and the second-order accuracy of the LBM is confirmed. We found that to attain better accuracy the LBM for the test problems requires a relatively small time step Δt and $\Delta t = 10^{-4}$ is a proper choice. Since the Chapman-Enskog analysis shows that this kind of complex-valued LBM is only the direct *translation* of the classical LBM in complex-valued function, the LBM can be applied directly to other complex evolutionary equations or real ones with complex-valued solutions.

Although the preliminary work in this paper shows that the classical LBM has also potentials to simulate complex-valued nonlinear systems, some problems still need to be solved, such as how to improve the accuracy and efficiency of complex LBM and that how does the complex LBM for CDE work when $\mathbf{u}$ is not constant.

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Appendix: Derivation of Macroscopic Equation

To derive the macroscopic equation (1), the Chapman-Enskog expansion in time and space is applied:

$$f_j = f_j^{eq} + \epsilon f_j^{(1)} + \epsilon^2 f_j^{(2)}, F = \epsilon F^{(1)}, \partial_t = \epsilon \partial_{t_1} + \epsilon^2 \partial_{t_2}, \nabla = \epsilon \nabla_1, \quad (18)$$

where ϵ is the Knudsen number, a small number.

From Eqs(18), (4) and (5), it follows that

$$\sum_j f_j^{(k)} = 0 (k \geq 1), \quad \sum_j F_j^{(1)} = F^{(1)}, \quad \sum_j \mathbf{c}_j F_j^{(1)} = \lambda F^{(1)} \mathbf{u}, \quad (19)$$

where $F_j^{(1)} = \omega_j F^{(1)} (1 + \lambda \frac{\mathbf{c}_j \cdot \mathbf{u}}{c_s^2})$ and λ is a parameter specified later.

Applying the Taylor expansion and Eq.(18) to Eq.(2), we have

$$O(\epsilon) : D_{1j} f_j^{eq} = -\frac{1}{\tau \Delta t} f_j^{(1)} + F_j^{(1)}, \quad (20)$$

$$O(\epsilon^2) : \partial_{t_2} f_j^{eq} + D_{1j} f_j^{(1)} + \frac{\Delta t}{2} D_{1j}^2 f_j^{eq} = -\frac{1}{\tau \Delta t} f_j^{(2)}. \quad (21)$$

where $D_{1j} = \partial_{t_1} + \mathbf{c}_j \cdot \nabla_1$.

Applying Eq.(20) to the left side of Eq.(21), we can rewrite Eq.(21) as

$$\partial_{t_2} f_j^{eq} + (1 - \frac{1}{2\tau}) D_{1j} f_j^{(1)} + \frac{\Delta t}{2} D_{1j} F_j^{(1)} = -\frac{1}{\tau \Delta t} f_j^{(2)}. \quad (22)$$

Summing Eq.(20) and Eq.(22) over j and using Eq.(4) and Eq.(19), we have

$$\partial_{t_1} \phi + \nabla_1 \cdot (\phi \mathbf{u}) = F^{(1)}, \quad (23)$$

$$\partial_{t_2} \phi + (1 - \frac{1}{2\tau}) \nabla_1 \cdot \sum_j \mathbf{c}_j f_j^{(1)} + \frac{\Delta t}{2} (\partial_{t_1} F^{(1)} + \nabla_1 \cdot (\lambda F^{(1)} \mathbf{u})) = 0. \quad (24)$$

Since $\mathbf{u}$ is a constant vector, using Eqs (20), (4), (19) and (23), we have

$$\begin{aligned} \sum_j \mathbf{c}_j f_j^{(1)} &= -\tau \Delta t \sum_j \mathbf{c}_j (D_{1j} f_j^{eq} - F_j^{(1)}) \\ &= -\tau \Delta t (\partial_{t_1} (\phi \mathbf{u}) + \nabla_1 \cdot (\phi \mathbf{u} \mathbf{u} + c_s^2 \phi \mathbf{I}) - \lambda F^{(1)} \mathbf{u}) \\ &= -\tau \Delta t (\mathbf{u} (\partial_{t_1} \phi + \nabla_1 \cdot (\phi \mathbf{u})) + c_s^2 \nabla_1 \phi - \lambda F^{(1)} \mathbf{u}) \\ &= -\tau \Delta t (c_s^2 \nabla_1 \phi + (1 - \lambda) F^{(1)} \mathbf{u}). \end{aligned} \quad (25)$$

Then substituting Eq.(25) into Eq.(24), we obtain

$$\partial_{t_2} \phi = \alpha \nabla_1^2 \phi + \Delta t (\tau - \frac{1}{2} - \lambda \tau) \nabla_1 \cdot (F^{(1)} \mathbf{u}) - \frac{\Delta t}{2} \partial_{t_1} F^{(1)}. \quad (26)$$

where $\alpha = c_s^2 (\tau - \frac{1}{2}) \Delta t$. Therefore, combining Eq.(26) with Eq.(23) and taking $\lambda = \frac{\tau - \frac{1}{2}}{\tau}$, we have

$$\partial_t \phi + \nabla \cdot (\phi \mathbf{u}) = \alpha \nabla^2 \phi + F - \frac{\Delta t}{2} \epsilon \partial_{t_1} F. \quad (27)$$

Neglecting the last term in the right side of Eq.(27), the CDE (1) is recovered. If we use the LB scheme proposed in Ref.[6], this term can be fully eliminated.