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Efficient lattice Boltzmann models for the Kuramoto–Sivashinsky equation

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In this work, we improve the accuracy and stability of the lattice Boltzmann model for the Kuramoto–Sivashinsky equation proposed in [1]. This improvement is achieved by controlling the relaxation time, modifying the equilibrium state, and employing more and higher lattice speeds, in a manner suggested by our analysis of the Taylor-series expansion method. The model's enhanced stability enables us to use larger time increments, thereby more than compensating for the extra computation required by the high lattice speeds. Furthermore, even though the time increments are larger than those of the previous scheme, the same level of accuracy is maintained because of the smaller truncation error of the new scheme. As a result, total performance with the new scheme on the D1Q7 lattice is improved by 92% compared to the original scheme on the D1Q5 lattice.

1. Introduction

The Kuramoto–Sivashinsky (KS) equation is well known to reproduce a variety of chaotic phenomena caused by intrinsic instability such as the unstable behavior of laminar flame fronts [2,3], thin-water-film flow on a vertical wall [4], and persistent wave propagation through a reaction-diffusion system [5]. For space X and time T, the KS equation for a quantity ρ is

$$\partial_T \rho + \rho \partial_X \rho = -\partial_X^2 \rho - \partial_X^4 \rho. \tag{1}$$

The second term on the left-hand side is the nonlinear advection term, while the first and second terms on the right-hand side are the production and hyperdiffusion terms, respectively. Examining the relationship between those terms, Holmes [6] found that the KS equation exhibits basic properties of turbulent flow, and indeed corresponds to the equation for the fluctuating velocity derived from the Navier–Stokes equation. Accordingly, the KS equation is often used to explore basic features of chaotic systems.

The lattice Boltzmann (LB) method was originally developed from models of lattice-gas cellular automata, and is based on principles of kinetic theory [7–9]. The ensemble of particle states is described by a distribution function which evolves through the particles' advection and collision process, thereby establishing the hydrodynamics. In addition to the hydrodynamic degrees of freedom, the model's kinetic modes depend on higher moments of the distribution function and give rise to peculiar features of the LB method, which are also beneficial for more detailed numerical modeling.

In the last decade, a number of LB models for nonlinear spatiotemporal systems have been developed [1,10–15]. In a previous study [1], LB models for nonlinear equations, such as the Burgers', Korteweg-de Vries, and Kuramoto–Sivashinsky (KS) equations, were derived using both the Chapman–Enskog and Taylor-series expansion methods [16,17] consistently. For simulating the long-time behavior of these chaotic equations accurately, however, the LB models thus derived require substantial computational time. Moreover, whereas the relaxation time τ in the LB model for the Navier–Stokes equation has a clear relationship to the viscosity, the role and optimized value of τ for the KS equation is not at all clear, and its value had to be set by trial and error. In this work, remedies for both of these issues are investigated using the Taylor-series expansion method, which allows for easy analysis of higher-order effects in the hydrodynamic equations.

This paper is organized as follows: In Section 2, we present a way to improve the LB model for the KS equation. In Section 3, we test the LB model thereby derived by comparisons with analytic solutions and with the previous model. In Section 4, we summarize the results of this study and present conclusions.

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Table 1
Moments of w_i.

Order of moments	$w_i^{(0)}$	$w_i^{(1)}$	$w_i^{(2)}$	$w_i^{(4)}$
0	1	0	0	0
1	0	1	0	0
2	0	0	1	0
3	0	0	0	0
4	0	0	0	1

Table 2
Coefficients of moments.

$\mathcal{J}$:	$\beta/2\alpha$
$\mathcal{K}$:	$-2\beta(\mathcal{T}_1+1)/\{\alpha^2(\mathcal{T}_2+1)\}$
$\mathcal{M}$:	$-24\beta(\mathcal{T}_1+1)/\{\alpha^4(\mathcal{T}_4+1)\}$

2. Improved lattice Boltzmann models for the Kuramoto–Sivashinsky equation

With discrete lattice velocities c_i and the relaxation time τ, the LB equation for the discrete distribution function f_i is given by:

$$f_i(x+c_i\Delta t, t+\Delta t) - f_i(x,t) = -\frac{f_i - f_i^{eq}}{\tau}. \tag{2}$$

Here f_i^{eq} is the local equilibrium state whose form for the KS equation, Eq. (1), was found in prior work [1] to be

$$f_i^{eq} = \rho\left(w_i^{(0)} + \mathcal{K}w_i^{(2)} + \mathcal{M}w_i^{(4)}\right) + \rho^2\mathcal{J}w_i^{(1)}, \tag{3}$$

where $\rho = \sum_i f_i$ and where the weights w_i have moments shown in Table 1. Explicit forms for these weights are presented in Appendix A. The quantities $\mathcal{K}$, $\mathcal{M}$, and $\mathcal{J}$ are given in Table 2, where we have defined $\mathcal{T}_i = \sum_{n=1}^{\infty}\left(1-\frac{1}{\tau}\right)^n\left[(n+1)^i - n^i\right]$. For $\tau > 1/2$ these are

$$\begin{aligned}
\mathcal{T}_1 &= \tau - 1\\
\mathcal{T}_2 &= 2\tau^2 - \tau - 1\\
\mathcal{T}_3 &= 6\tau^3 - 6\tau^2 + \tau - 1\\
\mathcal{T}_4 &= (\tau-1)\left(24\tau^3 - 12\tau^2 + 2\tau + 1\right).
\end{aligned} \tag{4}$$

The characteristic lattice speed $|c|$, which is dimensioned in lattice units, is assumed to be one and not explicitly written in what follows.

We use the Taylor-series expansion method for a small nondimensional parameter ϵ, with the scaling assumptions $\Delta x/L = \epsilon$ and $\Delta t/T = \epsilon^m$ for $m > 1$, and we assume that $L\partial_x$ and $T\partial_t$ are order unity, where L and T are macroscopic length and time scales. By summing over i in Eq. (2), one obtains [1],

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= -\mathcal{J}\frac{\partial\rho^2}{\partial x} + \frac{\Delta t}{2!}\mathcal{K}\frac{\partial^2\rho}{\partial x^2}\frac{\mathcal{T}_2+1}{\mathcal{T}_1+1} + \frac{(\Delta t)^3}{4!}\mathcal{M}\frac{\partial^4\rho}{\partial x^4}\frac{\mathcal{T}_4+1}{\mathcal{T}_1+1}\\
&\quad + \mathcal{O}\left(\frac{\partial^5\rho}{\partial x^5}, \frac{\partial^2\rho^2}{\partial x\partial t}, \frac{\partial^2\rho}{\partial t^2}\right).
\end{aligned} \tag{5}$$

The last term on the right-hand side is regarded as the truncation error for the KS equation.

In a simulation, the physical space X and physical time T are scaled with parameters α and β from the corresponding coordinates in lattice units, x and t, as follows

$$\begin{aligned}
X &= \alpha x\\
T &= \beta t.
\end{aligned} \tag{6}$$

The increments of physical space and time are therefore $\Delta X = \alpha$ and $\Delta T = \beta$. Taking this into account, it is straightforward to see that Eq. (1) can be derived from Eq. (5) with the choices of $\mathcal{J}$, $\mathcal{K}$ and $\mathcal{M}$ given in Table 2.

2.1. Strategy

It is worth highlighting several features of the above formalism:

- The requirements for the weights set forth in Table 1 can be satisfied with at least 5 lattice speeds, so D1Q5 would work.
- Higher moments than those shown in Table 1 impact only the truncation error in Eq. (5).
- As long as $\mathcal{K}$, $\mathcal{M}$, and $\mathcal{J}$ are as given in Table 2, the relaxation time does not influence the leading order terms in Eq. (5), but only the truncation error.

Due to the first point above, we adopt the D1Q5 lattice in this paper as our "basic scheme." Due to the second and third points, we see that by using more lattice speeds than the basic scheme and by varying the relaxation time, we may enhance accuracy while retaining stability. Although the increased number of speeds will require additional computation, if the time increments for achieving the same accuracy can be increased significantly, the total computational cost will be improved.

2.2. Analysis

According to our basic scheme, the leading truncation error term at order β^0 of Eq. (5) is the sixth spatial derivative term whose coefficients involve $\mathcal{K}$ and $\mathcal{M}$. By straightforward algebra, we find that this error term is

$$\left\{\frac{\alpha^4(\mathcal{T}_6+1)}{90(\mathcal{T}_2+1)} - \frac{\alpha^2(\mathcal{T}_6+1)}{6(\mathcal{T}_4+1)}\right\}\frac{\partial^6\rho}{\partial X^6}, \tag{7}$$

where we have substituted the forms of $\mathcal{K}$ and $\mathcal{M}$ from Table 2. Similarly, the truncation error terms at order β of Eq. (5) are those involving $\partial^2\rho/\partial t^2$, $\partial^3\rho/\partial t\partial x^2$, and $\partial^5\rho/\partial t\partial x^4$, whose coefficients also involve $\mathcal{K}$ and $\mathcal{M}$. By utilizing the leading order result, Eq. (1), these explicit forms are derived as

$$\begin{aligned}
&\beta\left\{\frac{\mathcal{T}_2+1}{2(\mathcal{T}_1+1)} - \frac{\mathcal{T}_3+1}{\mathcal{T}_2+1}\right\}\frac{\partial^4\rho}{\partial X^4}\\
&\quad+\beta\left\{\frac{\mathcal{T}_2+1}{\mathcal{T}_1+1} - \frac{\mathcal{T}_3+1}{\mathcal{T}_2+1} - \frac{\mathcal{T}_5+1}{\mathcal{T}_4+1}\right\}\frac{\partial^6\rho}{\partial X^6}.
\end{aligned} \tag{8}$$

In the derivation process of Eqs. (7) and (8), advection terms, namely those terms including ρ^2, are not taken into account for the sake of simplicity.

In order to remove the second term in Eq. (7) for the D1Q7 lattice, the following δf_i^{eq} is added to f_i^{eq} of Eq. (3),

$$\delta f_i^{eq} = \frac{120(\mathcal{T}_1+1)\beta}{(\mathcal{T}_4+1)\alpha^4}\rho w_i^{(6)}, \tag{9}$$

where $w_i^{(6)}$ is defined in Eq. (A.5).

In similar fashion, to remove the fourth derivative term in Eq. (8), the following $\delta\mathcal{M}$ is added to $\mathcal{M}$ in Table 2,

$$\delta\mathcal{M} = -\frac{24\beta^2(\mathcal{T}_1+1)}{\alpha^4(\mathcal{T}_4+1)}\left(\frac{\mathcal{T}_2+1}{2(\mathcal{T}_1+1)} - \frac{\mathcal{T}_3+1}{\mathcal{T}_4+1}\right). \tag{10}$$

The remaining error terms in Eqs. (7) and (8) are then

$$\left\{\frac{\alpha^4(\mathcal{T}_6+1)}{90(\mathcal{T}_2+1)} + \beta\left(\frac{\mathcal{T}_2+1}{\mathcal{T}_1+1} - \frac{\mathcal{T}_3+1}{\mathcal{T}_2+1} - \frac{\mathcal{T}_5+1}{\mathcal{T}_4+1}\right)\right\}\frac{\partial^6\rho}{\partial X^6}. \tag{11}$$

If this coefficient of the sixth derivative is positive, the system is very likely to be stable since the coefficient of the fourth derivative is negative. For $\tau = 1$, this condition can be written as

$$\frac{\alpha^4}{90} \geq \beta. \tag{12}$$

Thus, when β is not sufficiently small, an instability occurs. When τ is increased, however, this condition on β is weakened, since the

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