COMPUTER METHODS IN MATERIALS SCIENCE

2020, vol. 20, no. 4, 173–184
https://doi.org/10.7494/cmms.2020.4.0732

An accuracy analysis of the cascaded lattice Boltzmann method for the 1D advection-diffusion equation

Robert Straka[1,2*], Keerti V. Sharma[3]

[1] AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, Department of Heat Engineering and Environment Protection, al. Mickiewicza 30, 30-059, Krakow, Poland.

[2] Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Trojanova 13, 120 00, Praha 2, Czech Republic.

[3] Center of Innovation for Flow Through Porous Media, High Bay Research Facility, University of Wyoming, 651 N 19th street, Laramie, WY 82072, United States of America.

Abstract

We analyze higher order error terms in a modified partial differential equation of a cascaded lattice Boltzmann method (CLBM) for one conservation law – the advection-diffusion equation. To inspect the behavior of the error terms we derived an equivalent finite difference equation (EFDE), this approach is different from other techniques like the Chapman-Engskog expansion, equivalent partial differential equations or the Maxwell iteration used in the literature. The resulting EFDE is obtained from the recurrence formulas of the lattice Boltzmann equations for the CLBM and is subsequently analyzed by standard analytical techniques. We have found relations of the LBM parameters which could cancel some of the higher order terms, making the method more accurate. The detailed derivation of the EFDE and higher order terms' pre-factors is the main result of this paper. The resulting explicit form of the error terms are derived and presented.

Keywords: cascaded thermal lattice Boltzmann method, high order analysis, advection-diffusion equation, equivalent finite difference equation

1. Introduction

The cascaded lattice Boltzmann method emerged quite recently (Geier, 2006) and is slowly gaining attention within the LBM community (De Rosis, 2017; Fei & Luo, 2018; Fučík et al., 2018; Hajabdollahi & Premnath, 2018). The CLBM itself can be seen as a multiple relaxation time (MRT) scheme with non-standard collision matrix (Asinari, 2008). This matrix contains macroscopic velocities (i.e. it is not constant as in the case of classical MRT methods) (Asinari, 2008), making the implementation of the CLBM more complicated compared to single relaxation time (SRT) BGK or MRT methods (Geier et al., 2015). It is not only the computer implementation of the CLBM that is more complex, but also the analysis of the resulting partial differential equations reproduced by the CLBM is much more complicated in this case (Sharma et al., 2017). The analysis of the LBM is often performed up to the second order which is enough to inspect the hydrodynamic solved by the scheme and higher order analysis is left unsolved. The reason for that is quite obvious – the higher the order, the more complicated relations appear during the analysis when various

* Corresponding author: strakrob@gmail.com
ORCID ID's: 0000-0002-6479-7691 (R. Straka), 0000-0002-1262-5476 (K.V. Sharma)

techniques are used (Geier et al., 2015). The higher order analysis is quite rare even for the SRT and MRT methods (Dong et al., 2010; Ginzburg, 2012; Holdych et al., 2004; Zhao, 2013). Recently Geier et al. published 4th order analysis of the cumulant LBM for the Navier-Stokes equations (Geier & Pasquali, 2018; Geier et al., 2017). The cascaded scheme is related to the cumulants but they are not the same (Geier et al., 2015). From the techniques which can be found in the literature; Chapman–Enskog (Chen & Doolen, 1998), recurrence equations analysis (Ginzburg, 2012), equivalent partial differential equations (Dubois, 2008; Geier et al., 2015), Maxwell iterations (Zhao & Yong, 2017), Taylor expansion (Holdych et al., 2004) we used the one proposed by Suga (2010). Suga used this technique to check the error terms in the SRT-BGK LBM applied to a diffusion problem (Suga, 2009, 2010) and to derive more accurate finite difference schemes (Suga, 2006).

The paper is organized as follows; first the general recurrence equations for distribution functions with general collision matrix are derived, from these equations the EFDE is obtained and we proceed to the Taylor expansion of the EFDE. We end up with an equivalent partial differential equation (often called a modified partial differential equation) from which we can inspect higher order error terms and their pre-factors. These pre-factors are combinations of the relaxation times and lattice speed of sound, which can be carefully chosen to cancel or at least minimize higher order error terms. This issue is discussed further for the case of diffusion and advection-diffusion.

2. Cascaded lattice Boltzmann method

The lattice Boltzmann method is based on a simple equation which describes the evolution of the finite set of the q velocity distribution functions (DF) f_i on the finite lattice (set of points covering the computational domain) and can be generally written in the following form (using dimensionless lattice units i.e. $\Delta t = \Delta x = 1$):

$$\begin{aligned} &f_i(t+1, \mathbf{x}+\mathbf{c}_i) = \\ &f_i(t, \mathbf{x}) + \mathbf{A}_{ij}(f_j^{eq}(t, \mathbf{x}) - f_j(t, \mathbf{x})) = f_i^*(t, \mathbf{x}) \end{aligned} \tag{1}$$

where $i, j \in \{0, ..., q-1\}$; t and $\mathbf{x}$ are non-dimensional (in lattice units) time and position vector; $\mathbf{c_i}$ is a microscopic velocity associated with the DF; $\mathbf{A}$ is a collision matrix and f_i^{eq} is an equilibrium distribution function (EDF) for the i-th DF. The RHS of the above equation is called postcollision state and is abbreviated by f_i^*. The collision matrix and the EDF determine the macroscopic partial differential equation (PDE) solved by the Equation (1) called lattice Boltzmann equation (LBE). The EDF itself is a function of macroscopic variables, and collision matrix could be constant or could depend on the macroscopic velocity (this is the case for the CLBM). Macroscopic variables are obtained as moments[1] of the DF i.e.:

$$\phi = \sum_i f_i, \qquad \phi\mathbf{u} = \sum_i c_i f_i \tag{2}$$

where ϕ is scalar variable and $\mathbf{u}$ is macroscopic velocity.

In this paper we want to analyze error terms introduced by the CLBM when solving the advection-diffusion equation in 1D. We solve the following PDE with one unknown scalar variable $\phi(t, x)$, constant diffusion coefficient α and given velocity field $u(t, x)$:

$$\frac{\partial\phi}{\partial t} + \frac{\partial\phi u}{\partial x} = \alpha\frac{\partial^2\phi}{\partial x^2} \tag{3}$$

We also define the raw moments m_a and central moments κ_a:

$$m_a = \sum_i \mathbf{c}_i^a f_i, \qquad \kappa_a = \sum_i (\mathbf{c}_i - \mathbf{u})^a f_i \tag{4}$$

one can easily check the following relation[2]:

$$m_0 = \kappa_0 = \phi \tag{5}$$

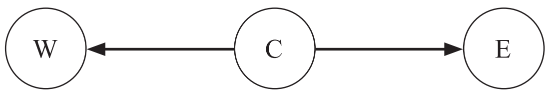

Fig. 1. D_1Q_3 lattice Boltzmann model of velocity set

Next we have to select the lattice and the velocity set, lattice in our case will be a grid of N equidistant points lying on the unit interval i.e. $x_i = (i + 0.5)\Delta x$ where $\Delta x = 1/N$ is the spatial step of the grid and $i \in 0, ..., N-1$. The velocity set we use is $\{c_0 = 0, c_1 = 1, c_2 = -1\}$, this LB model is called D_1Q_3 (see Fig. 1).

The collision in the cascaded LBM is performed in the central moment space:

$$\kappa_i^* = \kappa_i(t, x) - \omega_i(\kappa_i^{eq}(t, x) - \kappa_i(t, x)) \tag{6}$$

with ω_i being the relaxation frequency for i-th central moment. Due to the conservation of the ϕ we can

1 Here for the case of two conservation laws e.g. Navier–Stokes equations where φ denotes density of the fluid.
2 This is the only conserved moment – macroscopic variable – in our case.

choose $\omega_0 = 0$. Two remaining ω_1 and ω_2 controls the diffusion and the accuracy as we will show later (for simplicity of the derivation we use single relaxation time approach by setting $\omega_1 = \omega_2 = \omega$). The last thing which has to be established is the EDF, we use quadratic equilibrium defined by[3]:

$$\begin{pmatrix} \kappa_0^{eq} \\ \kappa_1^{eq} \\ \kappa_2^{eq} \end{pmatrix} = \begin{pmatrix} \phi \\ 0 \\ c_s^2 \phi \end{pmatrix} \tag{7}$$

where c_s is the speed of sound and – in the case of one conservation law – it can be set to certain values which maximizes the accuracy. Equilibria must also obey Equation (5):

$$m_0^{eq} = \kappa_0^{eq} = \phi \tag{8}$$

The post-collision state in central moments has to be transformed back to DF space to perform time update – so-called "streaming step". The procedure describing the transformation between DF, raw moments and central moments is detailed in the Appendix. The resulting LBE from Equation (1) has the following collision matrix:

$$\mathbf{A} = \begin{pmatrix} \omega u^2(t,x) & \omega(-1+u^2(t,x)) & \omega(-1+u^2(t,x)) \\ -\frac{\omega}{2}u(t,x)(u(t,x)+1) & \frac{\omega}{2}(2-u(t,x)-u^2(t,x)) & -\frac{\omega}{2}u(t,x)(u(t,x)+1) \\ \frac{\omega}{2}u(t,x)(1-u(t,x)) & \frac{\omega}{2}u(t,x)(1-u(t,x)) & \frac{\omega}{2}(2+u(t,x)-u^2(t,x)) \end{pmatrix} \tag{9}$$

We also use following abbreviations when referring to particular DF or macroscopic variables:

$$f_{C,x}^t = f_0(t,x), f_{E,x}^t = f_1(t,x), \\ f_{W,x}^t = f_2(t,x),\ \phi_x^t = \phi(t,x),\ u_x^t = u(t,x) \tag{10}$$

[3] The motivation for this choice is detailed in the Appendix.

3. Recurrence equations for CLBM

To proceed further we have to find recurrence equations for the DF. Let us take a look at the DF's postcollision state, using Equations (1) and (9) one can write down:

$$\begin{pmatrix} f_{C,x}^{t+1} \\ f_{E,x+1}^{t+1} \\ f_{W,x-1}^{t+1} \end{pmatrix} = \begin{pmatrix} f_{C,x}^{*,t} \\ f_{E,x}^{*,t} \\ f_{W,x}^{*,t} \end{pmatrix} = (\mathbf{I}-\mathbf{A}) \begin{pmatrix} f_{C,x}^{t} \\ f_{E,x}^{t} \\ f_{W,x}^{t} \end{pmatrix} + \mathbf{A} \begin{pmatrix} f_{C,x}^{eq,t} \\ f_{E,x}^{eq,t} \\ f_{W,x}^{eq,t} \end{pmatrix} \tag{11}$$

From the above equation the following recurrence rule can be deduced:

$$\begin{aligned} f_{j,x+n}^{t+m} &= \tilde{a}_{jj}(t+m-1,\ x+n-c_j)\phi_{x+n-c_j}^{t+m-1} + \\ &\sum_i (\tilde{a}_{ji}-\tilde{a}_{jj})(t+m-1,\ x+n-c_j) f_{i,x+n-c_j}^{t+m-1} + \\ &\sum_i a_{ji}(t+m-1,\ x+n-c_j) f_{i,x+n-c_j}^{eq,t+m-1} \end{aligned} \tag{12}$$

where $\tilde{a}_{ji}$ and a_{ji} are components of matrix $\mathbf{I} - \mathbf{A}$ and $\mathbf{A}$ respectively. Equation (12) will be used to derive EFDE for ϕ. Note that this form is fully general and can be used for other collision models like SRT-BGK or MRT (in that case the matrix $\mathbf{A}$ is constant and spatio-temporal dependence of a_{ij} and $\tilde{a}_{ij}$ vanishes).

The first iteration of Equation (12) yields:

$$f_{C,x}^{t+1} = (\omega-1)(f_{E,x}^t + f_{W,x}^t) + [1-\omega(c_s^2 + (u_x^t)^2)]\phi_x^t \tag{13}$$

$$\begin{aligned} f_{E,x}^{t+1} &= (\omega-1)(f_{C,x-1}^t + f_{W,x-1}^t) + \\ &\left[1-\omega+\frac{\omega}{2}(c_s^2 + u_{x-1}^t + (u_{x-1}^t)^2)\right]\phi_{x-1}^t \end{aligned} \tag{14}$$

$$\begin{aligned} f_{W,x}^{t+1} &= (\omega-1)(f_{C,x+1}^t + f_{E,x+1}^t) + \\ &\left[1-\omega+\frac{\omega}{2}(c_s^2 - u_{x+1}^t + (u_{x+1}^t)^2)\right]\phi_{x+1}^t \end{aligned} \tag{15}$$

Now we have to apply the Equations (12) and (2) several times to get rid of terms with DF, the resulting recurrence equation in terms of macroscopic variables reads:

$$\begin{aligned} \phi_x^{t+1} &= (1-\omega(c_s^2 + (u_x^t)^2)\phi_x^t + \\ &\left(1+\frac{\omega}{2}(-2+c_s^2 - u_{x+1}^t + (u_{x+1}^t)^2)\right)\phi_{x+1}^t + \\ &\left(1+\frac{\omega}{2}(-2+c_s^2 + u_{x-1}^t + (u_{x-1}^t)^2)\right)\phi_{x-1}^t + \\ &(\omega-1)\Bigg[(\omega-1)\phi_x^{t-2} + (1+\omega(-1+c_s^2+(u_x^{t-1})^2))\phi_x^{t-1} + \\ &\left(1+\frac{\omega}{2}(-c_s^2 - u_{x+1}^{t-1} + (u_{x+1}^{t-1})^2)\right)\phi_{x+1}^{t-1} + \\ &\left(1+\frac{\omega}{2}(-c_s^2 + u_{x-1}^{t-1} + (u_{x-1}^{t-1})^2)\right)\phi_{x-1}^{t-1}\Bigg] \end{aligned} \tag{16}$$

To make final analysis a bit easier we also assume constant velocity field $u(t, x) = u$ and express the EFDE in terms of time steps and lattice steps[4]:

$$
\begin{aligned}
&\phi_x^{t+\Delta t} = (1-\omega(c_s^2+u^2))\phi_x^t + \\
&\left(1+\frac{\omega}{2}(-2+c_s^2-u+u^2)\right)\phi_{x+\Delta x}^t + \\
&\left(1+\frac{\omega}{2}(-2+c_s^2+u+u^2)\right)\phi_{x-\Delta x}^t + \\
&(\omega-1)\Big[(\omega-1)\phi_x^{t-2\Delta t} + (1+\omega(-1+c_s^2+u^2))\phi_x^{t-\Delta t} + \\
&\left(1+\frac{\omega}{2}(-c_s^2-u+u^2)\right)\phi_{x+\Delta x}^{t-\Delta t} + \\
&\left(1+\frac{\omega}{2}(-c_s^2+u+u^2)\right)\phi_{x-\Delta x}^{t-\Delta t}\Big]
\end{aligned} \tag{17}
$$

4. Modified partial differential equation for CLBM

Equation (17) describes equivalent finite difference scheme of the CLBM and its terms can be Taylor expanded in time and space up to fourth order ($o = 4$) by the following formula:

$$
\begin{aligned}
&\phi_{x+m\Delta x}^{t+n\Delta t} + O(\partial^{o+1}) = \\
&\phi_x^t + \sum_{k=1}^{o}\frac{1}{k!}\sum_{l=0}^{k}\binom{k}{l}(n\Delta t)^{k-l}(m\Delta x)^l\frac{\partial^k}{\partial t^{k-l}x^l}\phi_x^t
\end{aligned} \tag{18}
$$

The result of the above operation is the following modified partial differential equation for the evolution of ϕ:

$$
\begin{aligned}
&\frac{\partial\phi}{\partial t} = \Delta t\left(\frac{3}{2}-\frac{2}{\omega}\right)\frac{\partial^2\phi}{\partial t^2} + \Delta t^2\left(-\frac{7}{6}+\frac{2}{\omega}-\frac{1}{\omega^2}\right)\frac{\partial^3\phi}{\partial t^3} + \\
&\Delta t^3\left(\frac{5}{8}-\frac{7}{6\omega}+\frac{1}{2\omega^2}\right)\frac{\partial^4\phi}{\partial t^4} - \frac{\Delta x}{\Delta t}\frac{\partial\phi u}{\partial x} + \Delta x\left(1-\frac{1}{\omega}\right)\frac{\partial^2\phi u}{\partial t\partial x} + \\
&\frac{\Delta x^2}{\Delta t}\left(-\frac{c_s^2}{2}+\frac{c_s^2}{\omega}-\frac{u^2}{2}+\frac{u^2}{\omega}\right)\frac{\partial^2\phi}{\partial x^2} - \frac{\Delta x^3}{6\Delta t}\frac{\partial^3\phi u}{\partial x^3} + \\
&\Delta t\Delta x\left(-\frac{1}{2}+\frac{1}{2\omega}\right)\frac{\partial^3\phi u}{\partial t^2\partial x} + \Delta t^2\Delta x\left(\frac{1}{6}-\frac{1}{6\omega}\right)\frac{\partial^4\phi u}{\partial t^3\partial x} + \\
&\Delta x^2\left(\frac{c_s^2}{2}+\frac{1}{\omega^2}-\frac{1}{\omega}-\frac{c_s^2}{2\omega}+\frac{u^2}{2}-\frac{u^2}{2\omega}\right)\frac{\partial^3\phi}{\partial t\partial x^2} + \\
&\Delta x^3\left(\frac{1}{6}-\frac{1}{6\omega}\right)\frac{\partial^4\phi u}{\partial t\partial x^3} + \\
&\frac{\Delta x^4}{\Delta t}\left(-\frac{c_s^2}{24}+\frac{c_s^2}{12\omega}-\frac{u^2}{24}+\frac{u^2}{12\omega}\right)\frac{\partial^4\phi}{\partial x^4} + \\
&\Delta t\Delta x^2\left(-\frac{c_s^2}{4}-\frac{1}{2\omega^2}+\frac{1}{2\omega}+\frac{c_s^2}{4\omega}-\frac{u^2}{4}+\frac{u^2}{4\omega}\right)\frac{\partial^4\phi}{\partial t^2\partial x^2}
\end{aligned} \tag{19}
$$

To get rid of mixed and temporal derivatives we recurrently substitute them using appropriate derivatives of the Equation (19) (this is different from the approach done by Suga (2010) where derivatives of the macroscopic advection-diffusion equation is used) and neglecting derivatives with order greater than four to obtain 4th order modified PDE:

$$
\begin{aligned}
&\frac{\partial\phi}{\partial t} + \frac{\Delta x}{\Delta t}\frac{\partial\phi u}{\partial x} = \frac{\Delta x^2}{\Delta t}C_2\frac{\partial^2\phi}{\partial x^2} + \\
&\frac{\Delta x^3}{\Delta t}C_3\frac{\partial^3\phi u}{\partial x^3} + \frac{\Delta x^4}{\Delta t}C_4\frac{\partial^4\phi}{\partial x^4}
\end{aligned} \tag{20}
$$

where coefficients C_2, C_3 and C_4 are given by:

$$
C_2 = c_s^2\left(\frac{1}{\omega}-\frac{1}{2}\right) \tag{21}
$$

$$
C_3 = \frac{(6-6\omega+\omega^2)(-1+3c_s^2+u^2)}{6\omega^2} \tag{22}
$$

$$
\begin{aligned}
C_4 &= (\omega-2)\frac{(12-12\omega+\omega^2)}{24\omega^3} \\
&\frac{(c_s^2-2c_s^4+6c_s^2u^2-3u^2+3u^4)-\omega^2c_s^4}{24\omega^3}
\end{aligned} \tag{23}
$$

The first term on the RHS of the Equation (20) describes the diffusion and the relation between diffusion coefficient α and lattice parameters c_s^2 and ω could be easily seen, we also see that we can set the desired diffusion by setting ω (which is usual practice) or by c_s^2 [5] (this way of setting diffusion is used in a thermal MRT scheme (Wang et al., 2013) and c_s^2 is hidden in parameter $a = 2c_s^2$ present in the equilibrium value of certain moments, other relaxation parameters are set to certain values which allows minimization of the error in advection and diffusion or enhance the stability of the scheme). The relation reads:

$$
\alpha = \frac{\Delta x^2}{\Delta t}c_s^2\left(\frac{1}{\omega}-\frac{1}{2}\right) = \frac{\Delta x^2}{\Delta t}\alpha_{lb} \tag{24}
$$

where α_{lb} denotes the diffusion coefficient in lattice units.

5. Analysis of high order error terms

Error terms described by coefficients C_3 and C_4 dictate the accuracy of the CLBM. While C_3 is in factor form and one can easily solve for a set of parameters which make this term equal to zero. C_4 is more complicated (due to the extra $\omega^2c_s^4$ term).

[4] Here Δt is equal to real time simulated by one iteration and Δx is the distance of two consecutive lattice sites.

[5] Usually the value of c_s^2 is set by solving lattice isotropy conditions (Wolf-Gladrow, 2005) and c_s^2 is then considered as the fixed value.

In fact we have three parameters ω, c_s^2 and u (velocity here is the lattice velocity which is related to the time step and physical velocity u_p by $u_p\Delta t = u\Delta x$). We have to choose Δt, Δx and set the parameters according to Equation (24) to obtain given diffusion coefficient. In any case, we have at least one free parameter left for the minimization of the error terms. In the case of pure advection ($\omega = 2$ and central moments are equilibrated in every time step) second and fourth order terms vanish and C_3 controls accuracy of the advection. In the case of pure diffusion the flow field vanishes $u = 0$, $C_3 = 0$ and C_4 reduces to:

$$C_4^{(d)} = (\omega-2)\frac{(12-12\omega+\omega^2)(c_s^2-2c_s^4)-\omega^2 c_s^4}{24\omega^3} \tag{25}$$

The C_3 term vanishes when:

$$\omega = 3 \pm \sqrt{3} \tag{26}$$

another choice is to set:

$$c_s^2 = \frac{1-u^2}{3} \tag{27}$$

in order to set appropriate diffusion coefficient, either both ω or c_s^2 is then evaluated from Equation (24). To nullify the $C_4^{(d)}$ term we have following choices:

$$\omega = \frac{-6+12c_s^2 \pm 2\sqrt{3}\sqrt{2-7c_s^2+6c_s^4}}{3c_s^2-1} \tag{28}$$

$$c_s^2 = \frac{12-12\omega+\omega^2}{24-24\omega+3\omega^2} \tag{29}$$

To investigate the C_4 term, we assume two different cases with parameters from Equations (26) and (27); first let $\omega = 3 \pm \sqrt{3}$ then the solution for $C_4 = 0$ reads:

$$c_s^2 = \frac{1+6u^2 \pm \sqrt{1+48u^2}}{2} \tag{30}$$

$$u = \pm\frac{\sqrt{3-6c_s^2 \pm \sqrt{3}\sqrt{3-16c_s^2+16c_s^4}}}{\sqrt{6}} \tag{31}$$

next let $c_s^2 = (1 - u^2)/3$, then the solution reads:

$$\omega = \frac{-1+7u^2 \pm \sqrt{1-12u^2+35u^4}}{u^2} \tag{32}$$

$$u = \pm\sqrt{2}\sqrt{\frac{1-\omega}{14-14\omega+\omega^2}} \tag{33}$$

$$u = \pm 1 \tag{34}$$

When we make plots of the above equations, we can observe the parameters for which the above terms are equal to zero as zero-level contours. In Figure 2 one can clearly see branches for $\omega = 3 \pm \sqrt{3}$ and c_s^2 close to the 1/3. The plot for the $C_4^{(d)}$ in Figure 3 is more complex, and we can observe that one can find c_s^2 for every useful ω i.e. for wide range of α_{lb} we can find both ω and c_s^2 for which $C_4^{(d)}$ will vanish and the scheme will be 4th order in diffusion. The same situation is visible in Figure 4 where the zero-level branch for c_s^2 is separate from 0 while u is increased. Contour plots for C_4 but in different variables are presented in Figures 5 and 6. Composite plot of absolute values of $|C_3| + |C_4|$ is shown in Figure 11. In Figures 7–10 we also present plots of curves described by Equations (30)–(33) for which the C_4 term vanish. These plots can serve as a hint for selecting the parameters which should control the diffusion and which should be set accordingly to discard C_3 and/or C_4 term.

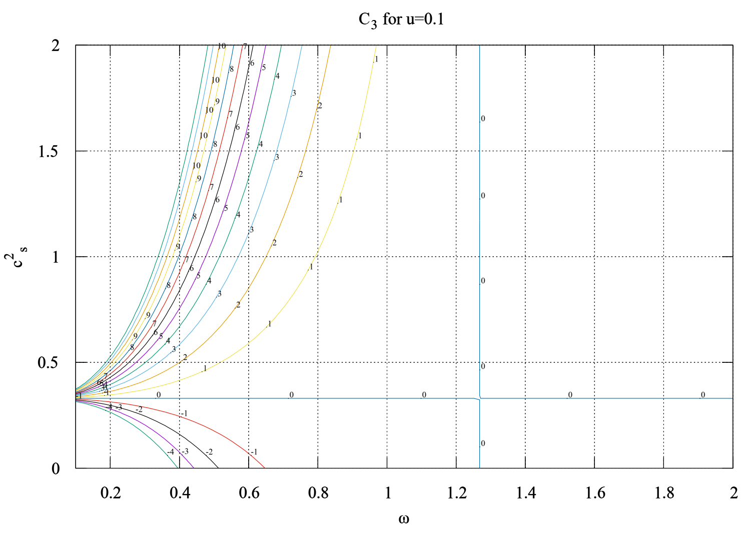

Fig. 2. Contours of the C_3 term as a function of ω and c_s^2 for $u = 0.1$ plots for $u = 0.01$, 0.001 are almost the same

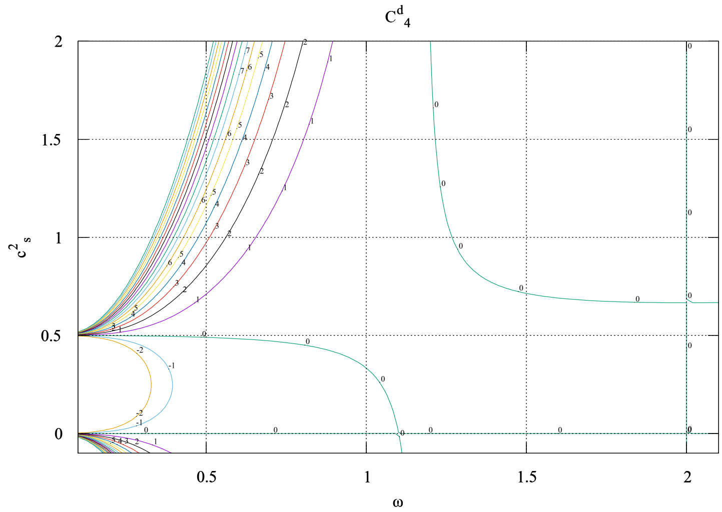

Fig. 3. Contours of the $C_4^{(d)}$ term as a function of ω and c_s^2

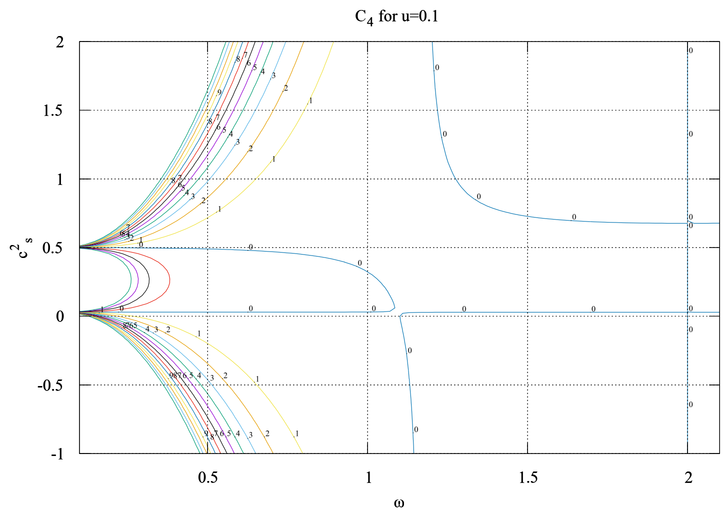

Fig. 4. Contours of the C_4 term as a function of ω and c_s^2 for $u = 0.1$ plots for $u = 0.01$, 0.001 are almost the same

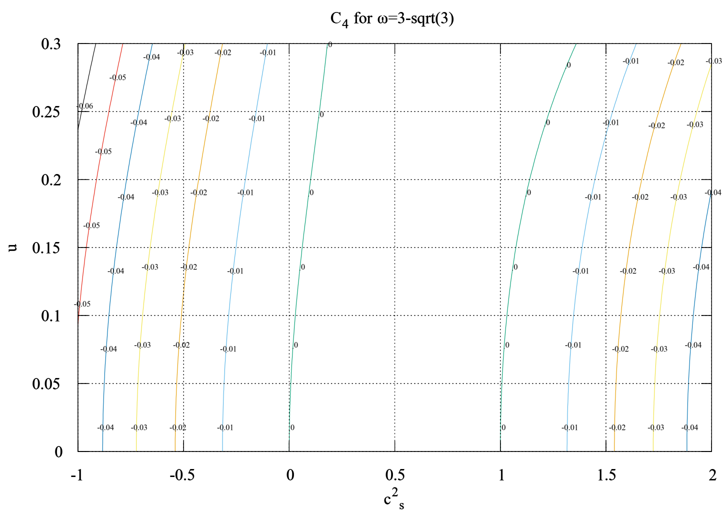

Fig. 5. Contours of the C_4 term as a function of c_s^2 and u for $\omega = 3 - \sqrt{3}$

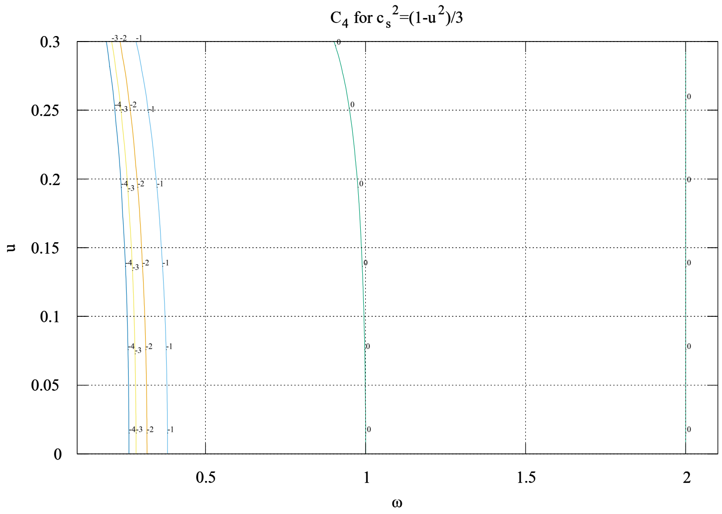

Fig. 6. Contours of the C_4 term as a function of ω and u for $c_s^2 = (1 - u^2)/3$

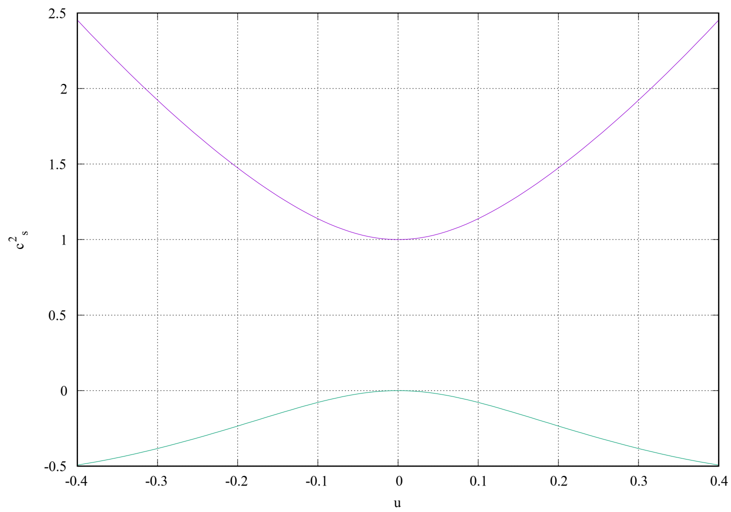

Fig. 7. Values of the c_s^2 from Eqution (30) as a function of u for $\omega = 3 \pm \sqrt{3}$

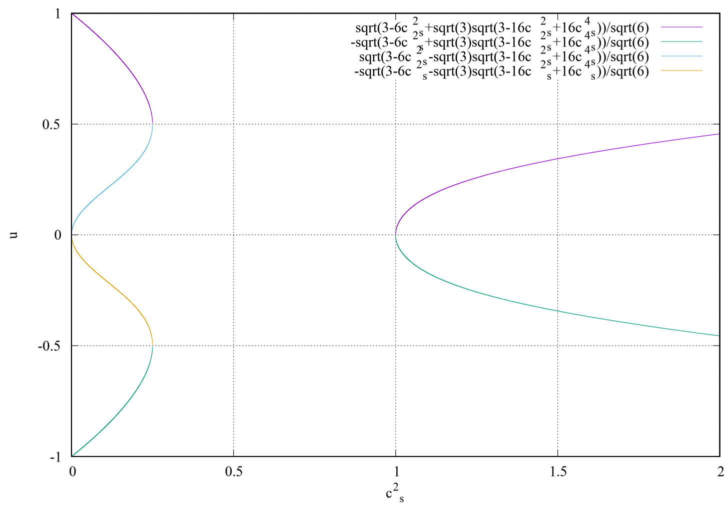

Fig. 8. Values of the u from Equation (31) as a function of c_s^2 for $\omega = 3 \pm \sqrt{3}$

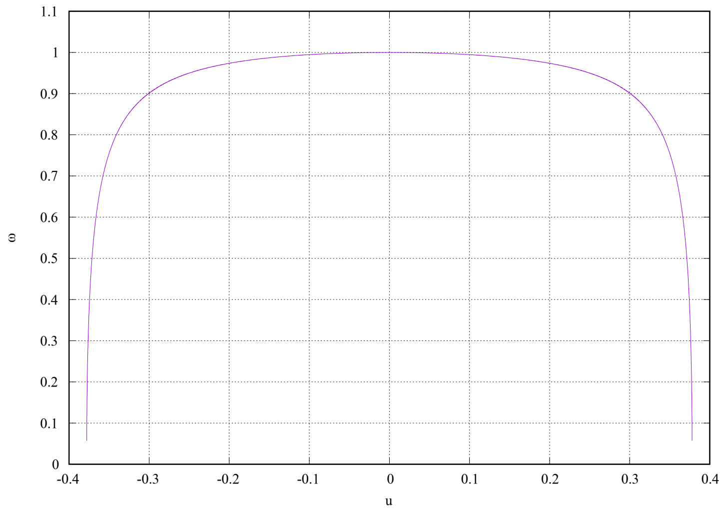

Fig. 9. Values of the ω from Equation (32) as a function of u for $c_s^2 = (1 - u^2)/3$

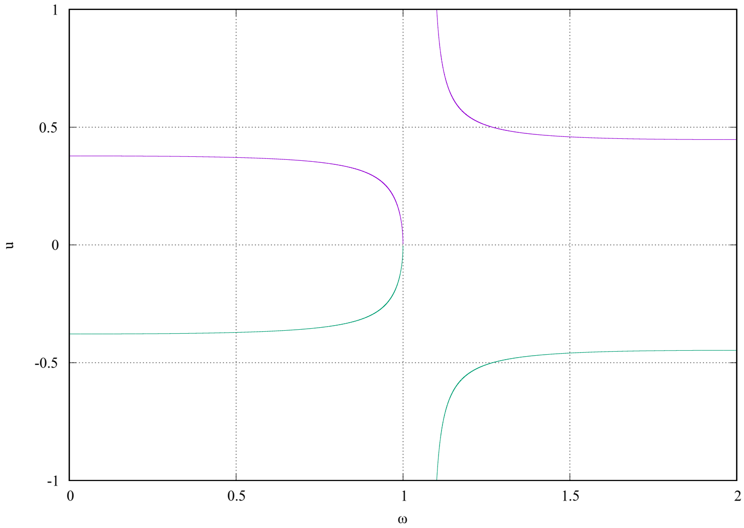

Fig. 10. Values of the u from Equation (33) as a function of ω for $c_s^2 = (1 - u^2)/3$

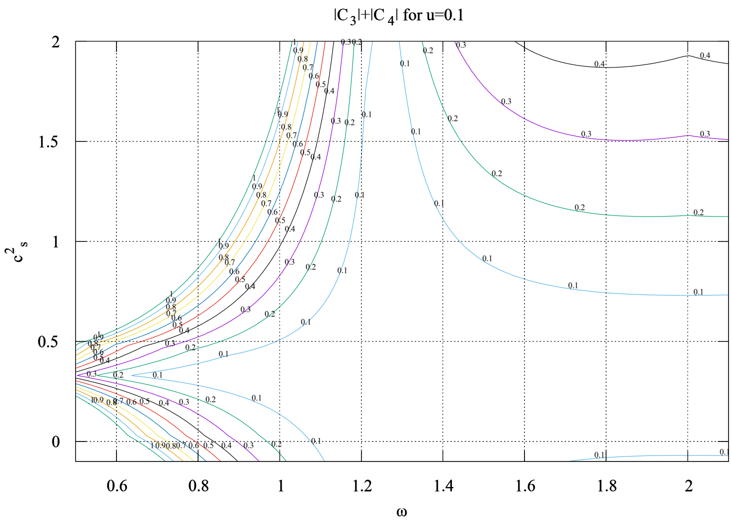

Fig. 11. Contours of the $|C_3| + |C_4|$ as a function of ω and c_s^2 for $u = 0.1$

The presented solutions describe the errors behavior in advection and diffusion. In simulations, one has to choose which term should be nullified or find an optimal set of parameters which makes both terms minimal keeping in mind that not all of the above solutions are admissible, the lattice velocity has to be less than c_s and $\omega \leq 2$ in order to ensure positivity of the diffusion coefficient.

Conclusion

The high order error terms of the cascaded LBM for the advection-diffusion equation in 1D were derived in the case of the SRT cascaded collision operator. We derived recursive equations for distribution functions and the equivalent finite difference equation is assembled from them. This EFDE is the starting point for the accuracy analysis of the scheme. The Taylor expansion yields pre-factors which control diffusion and higher order terms. For these pre-factors, we can find combinations of the LBM parameters which make those terms small or equal to zero. The detailed derivation of the collision matrix for D_1Q_3 and of recurrence equations is also described in the Appendices. The last Appendix describes the case of linear equilibrium and its influence of the resulting EFDE and pre-factors. The presented procedure could be extended to a higher dimension but must be performed algorithmically, there is no problem with constat collision matrices, non-constant matrices (resulting from e.g. cascaded or cumulant collision operators) are trickier in handling, but we are working on this aspect as well (Fučík & Straka, 2021).

Acknowledgement

R. Straka would like to acknowledge the support of the Czech Science Foundation project No. 18-09539S.

Appendix A. Construction of matrix A

The collision from Equation (1) is defined in distribution space i.e. in space of DF. In the case of SRT-BGK collision model, the matrix **A** is diagonal except for the first element, which is equal to zero. We can define the collision in moment space by transforming DF to moments. Moments have to be transformed back to DF after the collision as the streaming process is defined for DF and not for moments. The transformation of DF to moments can be described by the transformation matrix **M** constructed from the definition in Equation (4):

$$\mathbf{M}_{ij} = c_j^i \tag{A.1}$$

One can also use any linear combination of the raw moments as a basis for the moment space (d'Humières et al., 2002). In our case the matrix **M** reads:

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 & -1 \\ 0 & 1 & 1 \end{pmatrix} \tag{A.2}$$

and defines our moment space, where the collisions take place. Vectors of moments $\mathbf{m} = [m_0, m_1, m_2]^{\mathrm{T}}$ and DF $\mathbf{f} = [f_0, f_1, f_2]^{\mathrm{T}}$ are now conveniently defined as:

$$\mathbf{m} = \mathbf{Mf},\ \mathbf{f} = \mathbf{M}^{-1}\mathbf{m} \tag{A.3}$$

To perform collision in the previously defined moment space we also define relaxation matrices for SRT and MRT:

$$\mathbf{S}^{SRT} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega \end{pmatrix},\quad \mathbf{S}^{MRT} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega_1 & 0 \\ 0 & 0 & \omega_2 \end{pmatrix} \tag{A.4}$$

which allows us to express the collision in the moment space as:

$$\mathbf{m}^* = \mathbf{m} + \mathrm{S}^{\mathrm{SRT/MRT}}(\mathbf{m}^{eq} - \mathbf{m}) \tag{A.5}$$

where $\mathbf{m}^{eq} = \mathbf{Mf}^{eq}$ and after transformation back to DF we have:

$$\mathbf{f}^* = \mathbf{f} + \mathbf{M}^{-1}\mathrm{S}^{\mathrm{SRT/MRT}}\mathbf{M}(\mathbf{f}^{eq} - \mathbf{f}) \tag{A.6}$$

In order to perform collision in central moment space, we need also transformation matrices from moment space to central moment space **N** or direct transformation from DF to central moment space **K**, these are defined as follows:

$$\mathbf{N}_{ij} = \binom{i}{j}(-u(t,x))^{i-j},\quad \mathbf{K}_{ij} = (c_j - u(t,x))^i \tag{A.7}$$

in our case this gives us:

$$\begin{aligned} \mathbf{N} &= \begin{pmatrix} 1 & 0 & 0 \\ -u(t,x) & 1 & 0 \\ u^2(t,x) & -2u(t,x) & 1 \end{pmatrix} \\ \mathbf{K} &= \begin{pmatrix} 1 & 1 & 1 \\ -u(t,x) & 1-u(t,x) & -1-u(t,x) \\ u(t,x)^2 & (1-u(t,x))^2 & (-1-u(t,x))^2 \end{pmatrix} \end{aligned} \tag{A.8}$$

Now we can define a collision in a central moment space defined in Equation (6) as:

$$\mathbf{f}^* = \mathbf{f} + \mathbf{K}^{-1}\mathbf{S}^{\mathrm{SRT/MRT}}\mathbf{K}(\mathbf{f}^{eq} - \mathbf{f}) \tag{A.9}$$

from the above one can see that $\mathbf{A} = \mathbf{K}^{-1}\mathbf{S}^{\mathrm{SRT/MRT}}\,\mathbf{K}$.

Appendix B. Linear vs. quadratic equilibrium

The equilibria defined in Equation (7) contain quadratic terms in velocity. Transformation back to DF yields non-Galilean term in the second raw moment:

$$\mathbf{f}^{eq} = \mathbf{K}^{-1}\kappa^{eq} = \begin{pmatrix} (1-c_s^2)\phi(t,x) - \phi(t,x)u^2(t,x) \\ \frac{c_s^2\phi(t,x)}{2} + \frac{\phi(t,x)u(t,x)}{2} + \frac{\phi(t,x)u^2(t,x)}{2} \\ \frac{c_s^2\phi(t,x)}{2} - \frac{\phi(t,x)u(t,x)}{2} + \frac{\phi(t,x)u^2(t,x)}{2} \end{pmatrix} \tag{B.1}$$

$$\mathbf{m}^{eq} = \mathbf{N}^{-1}\kappa^{eq} = \begin{pmatrix} \phi(t,x) \\ \phi(t,x)u(t,x) \\ c_s^2\phi(t,x) + \phi(t,x)u^2(t,x) \end{pmatrix} \tag{B.2}$$

If we had used linear equilibrium in velocity i.e.:

$$\mathbf{f}^{eq,lin} = \begin{pmatrix} (1-c_s^2)\phi(t,x) \\ \frac{c_s^2\phi(t,x)}{2} + \frac{\phi(t,x)u(t,x)}{2} \\ \frac{c_s^2\phi(t,x)}{2} - \frac{\phi(t,x)u(t,x)}{2} \end{pmatrix} \tag{B.3}$$

we will obtain following equilibria for raw and central moments:

$$\mathbf{m}^{eq} = \begin{pmatrix} \phi(t,x) \\ \phi(t,x)u(t,x) \\ c_s^2\phi(t,x) \end{pmatrix}, \quad \kappa^{eq} = \begin{pmatrix} \phi(t,x) \\ 0 \\ c_s^2\phi(t,x) - \phi(t,x)u^2(t,x) \end{pmatrix} \tag{B.4}$$

Now the non-Galilean term appears in the second central moment. First iteration of Equation (12) with linear equilibrium yields:

$$f_{C,x}^{t+1} = (\omega-1)(f_{E,x}^t + f_{W,x}^t) + (1-\omega c_s^2)\phi_x^t \tag{B.5}$$

$$f_{E,x}^{t+1} = (\omega-1)(f_{C,x-1}^t + f_{W,x-1}^t) + \left[1-\omega+\frac{\omega}{2}(c_s^2 + u_{x-1}^t)\right]\phi_{x-1}^t \tag{B.6}$$

$$f_{W,x}^{t+1} = (\omega-1)(f_{C,x+1}^t + f_{E,x+1}^t) + \left[1-\omega+\frac{\omega}{2}(c_s^2 - u_{x+1}^t)\right]\phi_{x+1}^t \tag{B.7}$$

The resulting recurrence equation is as follows:

$$\begin{aligned} \phi_x^{t+1} &= (1-c_s^2\omega)\phi_x^t + \left[1+\omega\left(-1+\frac{c_s^2+u_{x-1}^t}{2}\right)\right]\phi_{x-1}^t + \\ &\left[1+\omega\left(-1+\frac{c_s^2-u_{x+1}^t}{2}\right)\right]\phi_{x+1}^t + \\ &(\omega-1)(1-\omega+c_s^2\omega)\phi_x^{t-1} + (\omega-1)^2\phi_x^{t-2} + \\ &(\omega-1)\left(1+\omega\frac{-c_s^2+u_{x-1}^{t-1}}{2}\right)\phi_{x-1}^{t-1} + \\ &(\omega-1)\left(1+\omega\frac{-c_s^2-u_{x+1}^{t-1}}{2}\right)\phi_{x+1}^{t-1} \end{aligned} \tag{B.8}$$

The diffusion term C_2 and C_3, $C_4^{(d)}$ and C_4 terms become:

$$C_2 = \frac{(\omega-2)(u+c_s^2)(u-c_s^2)}{2\omega} \tag{B.9}$$

$$C_3 = \frac{u(6-6\omega+\omega^2)(1-3c_s^2+2u^2)}{6\omega^2} \tag{B.10}$$

$$C_4^{(d)} = \frac{c_s^2(\omega-2)(2c_s^2-1)(12-12\omega+\omega^2)}{24\omega^3} \tag{B.11}$$

$$\begin{aligned} C_4 = (\omega-2)&\frac{(12-12\omega+\omega^2)}{24\omega^3} \\ &\frac{(-c_s^2+2c_s^4+4u^2-10c_s^2u^2+5u^4)}{24\omega^3} + \\ &\frac{c_s^4\omega^2-2c_s^2\omega^2u^2+u^2\omega^2}{24\omega^3} \end{aligned} \tag{B.12}$$

We can observe that using linear equilibrium yields diffusion which is velocity dependent, this fact was described by Chopard et al. (2009) and an appropriate correction was proposed there.

Appendix C. Detailed derivation of recurrence equatios

If we take a look at Equations (13)–(15) we can see that we need to get rid of DF on the RHS (the LHS will be summed later to obtain $\phi(t+1, x)$). We use recurrence rule in Equation (12) for their sum to obtain:

$$\begin{aligned}
&f_{C,x-1}^{t} + f_{W,x-1}^{t} + f_{E,x}^{t} + f_{W,x}^{t} + f_{C,x+1}^{t} + f_{E,x+1}^{t} = \\
&\phi_x^{t-1}(2-2\omega + c_s^2\omega + \omega(u_x^{t-1})^2) + \\
&\phi_{x-1}^{t-1}\left(2-\omega-\frac{c_s^2\omega}{2}+\frac{\omega u_{x-1}^{t-1}}{2}-\frac{\omega(u_{x-1}^{t-1})^2}{2}\right)+ \\
&\phi_{x+1}^{t-1}\left(2-\omega-\frac{c_s^2\omega}{2}-\frac{\omega u_{x+1}^{t-1}}{2}-\frac{\omega(u_{x+1}^{t-1})^2}{2}\right)+ \\
&(\omega-1)(f_{C,x-1}^{t-1} + f_{E,x-1}^{t-1} + f_{E,x}^{t-1} + f_{W,x}^{t-1} + f_{C,x+1}^{t-1} + f_{W,x+1}^{t-1}) + \\
&(2\omega-2)(f_{W,x-1}^{t-1} + f_{C,x}^{t-1} + f_{E,x+1}^{t-1})
\end{aligned} \tag{C.1}$$

Next we use the following substitutions in the above equation:

$$f_{C,x-1}^{t-1} = -f_{E,x-1}^{t-1} + \phi_{x-1}^{t-1} - f_{W,x-1}^{t-1} \tag{C.2}$$

$$f_{E,x}^{t-1} = -f_{W,x}^{t-1} + \phi_{x}^{t-1} - f_{C,x}^{t-1} \tag{C.3}$$

$$f_{C,x+1}^{t-1} = -f_{E,x+1}^{t-1} + \phi_{x+1}^{t-1} - f_{W,x+1}^{t-1} \tag{C.4}$$

which yields:

$$\begin{aligned}
&f_{C,x-1}^{t} + f_{W,x-1}^{t} + f_{E,x}^{t} + f_{W,x}^{t} + f_{C,x+1}^{t} + f_{E,x+1}^{t} = \\
&\phi_x^{t-1}(1-1\omega + c_s^2\omega + \omega(u_x^{t-1})^2) + \\
&\phi_{x-1}^{t-1}\left(1-\frac{c_s^2\omega}{2}+\frac{\omega u_{x-1}^{t-1}}{2}-\frac{\omega(u_{x-1}^{t-1})^2}{2}\right)+ \\
&\phi_{x+1}^{t-1}\left(1-\frac{c_s^2\omega}{2}-\frac{\omega u_{x+1}^{t-1}}{2}-\frac{\omega(u_{x+1}^{t-1})^2}{2}\right)+ \\
&(\omega-1)(f_{W,x-1}^{t-1} + f_{C,x}^{t-1} + f_{E,x+1}^{t-1})
\end{aligned} \tag{C.5}$$

The expansion of the last term gives us:

$$\begin{aligned}
&f_{W,x-1}^{t-1} + f_{C,x}^{t-1} + f_{E,x+1}^{t-1} = \\
&(3-2\omega)\phi_x^{t-2} + (2\omega-2)(f_{C,x}^{t-2} + f_{E,x}^{t-2} + f_{W,x}^{t-2}) = \\
&(3-2\omega)\phi_x^{t-2} + (2\omega-2)\phi_x^{t-2} = \phi_x^{t-2}
\end{aligned} \tag{C.6}$$

If the above Equations (C.5) and (C.6) are inserted into the first step of recurrence expansions (13)–(15) and resulting system of equations are summed we end up with the EFDE from the Equation (16).

References

Asinari, P. (2008). Generalized local equilibrium in the cascaded lattice Boltzmann method. *Physical Review E*, *78*(1), 016701. https://doi.org/10.1103/physreve.78.016701.

Chen, S., & Doolen, G. (1998). Lattice Boltzmann Method for fluid flows. *Annual Review of Fluid Mechanics*, *30*, 329–364. https://doi.org/10.1146/annurev.fluid.30.1.329.

Chopard, B., Falcone, J.L., & Latt, J. (2009). The lattice Boltzmann advection-diffusion model revisited. *The European Physical Journal Special Topics*, *171*(1), 245–249. https://doi.org/10.1140/epjst/e2009-01035-5.

d'Humières, D. (2002). Multiple-relaxation-time lattice Boltzmann models in three dimensions. *Philosophical Transactions of The Royal Socciety A: Mathematical, Physical and Engineering Sciences*, *360*(1792), 437–51. https://doi.org/10.1098/rsta.2001.0955.

De Rosis, A. (2017). Nonorthogonal central-moments-based lattice Boltzmann scheme in three dimensions. *Physical Review E*, *95*, 013310. https://doi.org/10.1103/PhysRevE.95.013310.

Dong, Y., Zhang, J., & Yan, G. (2010). A higher-order moment method of the lattice Boltzmann model for the conservation law equation. *Applied Mathematical Modelling*, *34*(2), 481–494. https://doi.org/10.1016/j.apm.2009.06.024.

Dubois, F. (2008). Equivalent partial differential equations of a lattice Boltzmann scheme. *Computers & Mathematics with Applications*, *55*(7), 1441–1449. https://doi.org/10.1016/j.camwa.2007.08.003.

Fei, L., & Luo, K.H. (2018). Cascaded lattice Boltzmann method for incompressible thermal flows with heat sources and general thermal boundary conditions. *Computers and Fluids*, *165*, 89–95. https://doi.org/10.1016/j.compfluid.2018.01.020.

Fučík, R., & Straka, R. (2021). Equivalent finite difference and partial differential equations for the lattice Boltzmann method. *Computers & Mathematics with Applications*, *90*, 96–103. https://doi.org/10.1016/j.camwa.2021.03.014

Fučík, R., Eichler, P., Straka, R., Pauš, P., Klinkovský, J., & Oberhuber, T. (2018). On optimal node spacing for immersed boundary-lattice Boltzmann method in 2D and 3D. *Computers & Mathematics with Applications*, *77*(4), 1144–1162. https://doi.org/10.1016/j.camwa.2018.10.045.

Geier, M.C. (2006). *Ab initio derivation of the cascaded lattice Boltzmann automaton* [PhD. Thesis]. University of Freiburg, Germany. https://freidok.uni-freiburg.de/data/2860/.

Geier, M., & Pasquali, A. (2018). Fourth order Galilean invariance for the lattice Boltzmann method. *Computers & Fluids*, *166*, 139–151. https://doi.org/10.1016/j.compfluid.2018.01.015.

Geier, M., Schönherr, M., Pasquali, A., & Krafczyk, M. (2015). The Cumulant lattice Boltzmann equation in three dimensions: Theory and validation. *Computers & Mathematics with Applications*, *70*(4), 507–547. https://doi.org/10.1016/j.camwa.2015.05.001.

Geier, M., Pasquali, A., & Schönherr, M. (2017). Parametrization of the cumulant lattice Boltzmann method for fourth order accurate diffusion Part I: Derivation and validation. *Journal of Computational Physics*, *348*, 862–888. https://doi.org/10.1016/j.jcp.2017.05.040.

Ginzburg, I. (2012). Truncation Errors, Exact and Heuristic Stability Analysis of Two-Relaxation-Times Lattice Boltzmann Schemes for Anisotropic Advection-Diffusion Equation. *Communications in Computational Physics*, *11*(5), 1439–1502. https://doi.org/10.4208/cicp.211210.280611a.

Hajabdollahi, F., & Premnath, K.N. (2018). Symmetrized Operator Split Schemes for Force and Source Modeling in Cascaded Lattice Boltzmann Methods for Flow and Scalar Transport. *Physical Review E*, *97*(6), 063303. https://doi.org/10.1103/PhysRevE.97.063303.

Holdych, D.J., Noble, D.R., Georgiadis, J.G., & Buckius, R.O. (2004). Truncation error analysis of lattice Boltzmann methods. *Journal of Computational Physics*, *193*(2), 595–619. https://doi.org/10.1016/j.jcp.2003.08.012.

Sharma, K.V., Straka, R., & Tavares, F.W. (2017). New Cascaded Thermal Lattice Boltzmann Method for Simulations of Advection-Diffusion and Convective Heat Transfer. *International Journal of Thermal Sciences*, *118*, 259–277. https://doi.org/10.1016/j.ijthermalsci.2017.04.020.

Suga, S. (2006). Numerical scheme obtained from lattice Boltzmann equations for advection diffusion equations. *International Journal of Modern Physics C*, *17*(11), 1563–1577. https://doi.org/10.1142/S0129183106010030.

Suga, S. (2009). Stability and accuracy of lattice Boltzmann schemes for anisotropic advection-diffusion equations. *International Journal of Modern Physics C*, *20*(4), 633–650. https://doi.org/10.1142/S0129183109013856.

Suga, S. (2010). An accurate multi-level finite difference scheme for 1D diffusion equations derived from the lattice Boltzmann method. *Journal of Statistical Physics*, *140*(3), 404–503. https://doi.org/10.1007/s10955-010-0004-y.

Wang, J., Wang, D., Lallemand, P., & Luo, L.-S. (2013). Lattice Boltzmann simulations of thermal convective flows in two dimensions. *Computers & Mathematics with Applications*, *65*(2), 262–286. https://doi.org/10.1016/j.camwa.2012.07.001.

Wolf-Gladrow, D.A. (2005). *Lattice-gas cellular automata and lattice Boltzmann models. An introduction*. Springer. https://doi.org/10.1007/b72010.

Zhao, F. (2013). Optimal relaxation collisions for lattice Boltzmann methods. *Computers & Mathematics with Applications*, *65*(2), 172–185. https://doi.org/10.1016/j.camwa.2011.06.005.

Zhao, W., & Yong, W.-A. (2017). Maxwell iteration for the lattice Boltzmann method with diffusive scaling. *Physical Review E*, *95*(3), 033311. https://doi.org/10.1103/PhysRevE.95.033311.