Commun. Comput. Phys.
doi: 10.4208/cicp.2014.m369

Vol. **17**, No. 5, pp. 1225-1245
May 2015

L_2 Convergence of the Lattice Boltzmann Method for One Dimensional Convection-Diffusion-Reaction Equations

Michael Junk[1] and Zhaoxia Yang[1,*]

[1] *FB Mathematik und Statistik, Universität Konstanz, Postfach D194, 78457 Konstanz, Germany.*

Received 11 November 2013; Accepted (in revised version) 17 June 2014

Abstract. Combining asymptotic analysis and weighted L_2 stability estimates, the convergence of lattice Boltzmann methods for the approximation of 1D convection-diffusion-reaction equations is proved. Unlike previous approaches, the proof does not require transformations to equivalent macroscopic equations.

AMS subject classifications: 65, 41, 76, 35

Key words: Lattice Boltzmann method, convection-diffusion-reaction equation, L_2 stability, L_2 convergence.

1 Introduction

In this article, we consider a variant of the lattice Boltzmann method for the solution of the convection-diffusion-reaction equation (for example, see [3, 8, 16, 18, 19]). The practical validity of the method has been investigated through formal consistency analysis (Chapman-Enskog expansion or asymptotic expansion) and numerical convergence studies. On top of that, stability properties have been checked by numerical tests and investigation of spectral properties (von Neumann stability analysis). While these investigations are all important in their own right, convergence results add further confidence to the method.

At this point, it could be argued that the accessibility of consistency and stability results automatically entails convergence due to a general theorem of von Neumann. However, a detailed revision of the required prerequisites shows that the standard convergence theory is based on a more specific notion of consistency and stability than the one available for lattice Boltzmann methods. As far as consistency is concerned, this is due to the fact that the lattice Boltzmann equation approximates a singularly perturbed

*Corresponding author. *Email addresses:* `michael.junk@uni-konstanz.de` (M. Junk), `zhaoxia.yang@uni-konstanz.de` (Z. Yang)

discrete velocity model with a coupling between discretization and perturbation parameters, leading to a more intricate behavior compared to discretizations of unperturbed differential equations. Also, the non-symmetry of the evolution matrix which describes the effect of a single lattice Boltzmann step renders the investigation of its eigenvalue structure useless for obtaining L_2-norm estimates which are employed in standard convergence proofs (of course, this does not reduce its importance in providing information on the stability of the solution for a fixed setting of the discretization parameters).

For these reasons, convergence proofs for lattice Boltzmann methods follow somewhat different strategies than in classical numerical analysis. As examples, we mention the work [7, 22] where convergence of lattice Boltzmann D1Q2 models is proved based on a technique which requires the equivalent moment equations. This technique is applicable for small systems in 1D but seems less efficient for higher dimensional cases, where the moment systems are much larger and cumbersome to set up.

Having all these aspects in mind, we can now formulate the aim of this paper: we want to present and advocate a different proof strategy which is based on the lattice Boltzmann equation itself and which extends to higher dimensions in a straightforward manner. As for the stability aspect, we will show that the results [1, 14] on stability of lattice Boltzmann methods for the Navier-Stokes equation can be extended to the case of the convection-diffusion-reaction equation. This stresses the universality of the approach. As a side effect, conditions on the discretization parameters (in the spirit of the CFL condition) will be found which guarantee convergence of the method in a particular case.

As for consistency, we employ asymptotic analysis and split the asymptotic description of the numerical solution into smooth and non-smooth parts. The smooth parts contain information on the solution of the convection-diffusion-reaction equation and possible errors which are of lower order in grid size and governed by known equations. The non-smooth part will be one order lower than the smooth error which allows us to reduce the smoothness assumptions on the data such as convection speed or reaction rate.

To demonstrate the basic ideas of the strategy, it is reasonable to restrict to 1D lattice Boltzmann schemes with simple periodic boundary conditions because, then, the proofs are particularly easy to display and examine. We hope that, in this way, the reader may understand the basic idea in each detail. Results for higher dimensional problems and non-periodic boundary conditions will appear in subsequent papers.

After presenting the basic equations in Section 2 and the consistency analysis in Section 3, stability results are summarized in Theorems 4.1, 4.2, and Theorem 5.3, where a priori estimates are obtained. The convergence results can be found in Section 5.

2 Lattice Boltzmann schemes in 1D

We consider a general one-dimensional convection-diffusion-reaction equation for some density $\rho:[0,T]\times\mathbb{R}\mapsto\mathbb{R}$,

$$\partial_t \rho + \partial_x (u\rho) = \nu \partial_x^2 \rho - \kappa \rho, \tag{2.1}$$

which involves a convection speed $u:[0,T]\times\mathbb{R}\mapsto\mathbb{R}$, a constant diffusivity ν and a reaction coefficient $\kappa:[0,T]\times\mathbb{R}\mapsto\mathbb{R}$. The problem is completed with an initial condition

$$\rho(0,x) = \phi(x), \quad x\in\mathbb{R} \tag{2.2}$$

and, for the considerations here, with an x-periodicity assumption on u,κ,ϕ which implies periodicity of the solution ρ.

To solve this one dimensional problem numerically, the lattice Boltzmann method is a feasible algorithm due to the fact that Eq. (2.1) can be seen as diffusive limit of a discrete velocity kinetic system with lattice Boltzmann structure. The detailed investigation of that limit can be carried out using the Chapman-Enskog [6,8,16] or the Hilbert expansion [9,10,23] (also called asymptotic analysis later).

The standard lattice Boltzmann method is based on an equi-distant mesh with nodes x_j and mesh size h as well as a uniform time step $\Delta t = h^2$. The n-th time level is given by $t_n = nh^2$. The lattice Boltzmann method is then written in the form

$$f_i(n+1, j+c_i) = f_i^{(c)}(n,j), \tag{2.3}$$

with

$$f_i^{(c)}(n,j) = f_i(n,j) + J_i(\boldsymbol{f}(n,j)) + h^2 g_i(n,j). \tag{2.4}$$

Eq. (2.3) describes the transport phase and Eq. (2.4) the collision phase of the algorithm. Here, $f_i(n,j)$ represent the particle distribution function at time level t_n and position x_j according to the particle velocity c_i. The vector $\boldsymbol{f}$ has f_i as components and forms a vector in $\mathbb{R}^N$ if there are N distinct particle velocities. Similarly, we use boldface notation for vectors like $\boldsymbol{f}^{(c)}$ or $\boldsymbol{g}$.

The collision operator J is of multiple relaxation type, namely $J = A(\boldsymbol{f}^{eq} - \boldsymbol{f})$ with a constant, diagonalizable matrix $A = M^{-1}\Gamma M \in \mathbb{R}^{N\times N}$ in which Γ is a diagonal matrix containing all the eigenvalues γ_i of A. f_i^{eq} is the equilibrium function defined by

$$f_i^{eq} = F_i^{eq}(\hat{\rho}) = w_i \hat{\rho}(1 + \theta h u c_i), \tag{2.5}$$

where the total density $\hat{\rho}$ is the summation of all f_i, i.e.

$$\hat{\rho} = \sum_{i=1}^{N} f_i. \tag{2.6}$$

The parameters w_i represent a reference equilibrium at zero velocity and unit density and θ is a fixed parameter which depends on the chosen set of discrete velocities c_i. The reaction term g_i may be implemented according to [8,16] as a source term

$$g_i(n,j) = w_i \kappa(t_n, x_j)\hat{\rho}(n,j), \quad \text{or} \quad g_i(n,j) = \frac{1}{N}\kappa(t_n, x_j)\hat{\rho}(n,j). \tag{2.7}$$

Actually, the reaction term can also be integrated into the equilibrium function [17]. Both treatments do not affect the accuracy order and do not show essential differences in the convergence proof either. However, they may affect the boundary conditions and the magnitude of the numerical error. For concreteness, we adopt the first choice in (2.7).

If all γ_i are equal, the matrix A is reduced to $\gamma_1 \boldsymbol{I}$ which corresponds to the so-called single relaxation BGK model [2]. The classical TRT model [8] employs two generally different eigenvalues. One can find examples of MRT models in [21] for D2Q5 and [23] for D3Q17.

Obviously, the proposed lattice Boltzmann schemes vary with the choice of c_i, w_i, M and Γ. This choice is structurally restricted by the condition, that the correct diffusive limit is obtained. The following two models will be considered in our convergence proof.

D1Q2 model

$$\begin{aligned} &c_i \in \{-1,1\} \quad \text{and} \quad w_1 = w_2 = \frac{1}{2}, \quad \theta = 1, \\ &M = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \Gamma = \begin{pmatrix} \gamma_1 & 0 \\ 0 & \gamma_2 \end{pmatrix}, \quad M^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}. \end{aligned} \tag{2.8}$$

D1Q3 models

$$\begin{aligned} &c_i \in \{0,-1,1\}, \quad w_1 = 1-2b, \quad w_2 = w_3 = b, \quad b \in \left(0, \frac{1}{2}\right), \quad \theta = \frac{1}{2b}, \\ &M = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -1 & 1 \\ -2 & 1 & 1 \end{pmatrix}, \quad \Gamma = \begin{pmatrix} \gamma_1 & 0 & 0 \\ 0 & \gamma_2 & 0 \\ 0 & 0 & \gamma_3 \end{pmatrix}, \quad M^{-1} = \frac{1}{6}\begin{pmatrix} 2 & 0 & -2 \\ 2 & -3 & 1 \\ 2 & 3 & 1 \end{pmatrix}. \end{aligned} \tag{2.9}$$

In both models, the role of the first eigenvalue γ_1 is somewhat special because, for any choice of $\boldsymbol{f}$, the vector $\boldsymbol{f} - \boldsymbol{f}^{eq}$ is orthogonal to the first row of M. As a consequence, the value of γ_1 has no influence on the outcome of the collision and, thus, can be chosen arbitrarily. Obviously in 1D, the MRT model is equivalent to the TRT model.

In case of the D1Q2 model without reaction and convection terms (only diffusion), Weiß [22] has transformed the lattice Boltzmann scheme into its equivalent moment system where $\boldsymbol{m} = M\boldsymbol{f}$ are the independent variables. He could show a weighted L_2-convergence. Dellecharie [7], however, has tried to construct those lattice Boltzmann schemes which are equivalent to a known explicit finite difference scheme for $\hat{\rho}$, so that L_∞ stability is guaranteed and convergence is achieved.

It should be noted that these two ideas are feasible due to the small system size (2×2) in 1D. However, when extending the considerations to the 2D or 3D case, the discrete velocity sets are considerably larger (e.g. D2Q9 with 9 directions and D3Q15 with 15). Then it is cumbersome to work with equivalent moment systems and associated difference schemes for $\hat{\rho}$.

Therefore, in this paper, we present a convergence proof, which operates directly and only on the original formulation of the lattice Boltzmann equation so that the transfer to higher dimensions is straight forward. The basic procedure is similar to Strang's classical approach [20], where convergence is obtained as a consequence of stability and consistency. We investigate consistency with the help of asymptotic analysis and apply the stability analysis in [14] to the 1D case.

3 Asymptotic analysis

Consistency analysis of the lattice Boltzmann method is carried out by means of the so-called asymptotic analysis which yields important information on the structure of the numerical solution order by order in grid size h. Another possibility, where the h-dependence is somewhat less transparent, is given by the Chapman-Enskog expansion [5]. We refer to [10, 13] as an example of a detailed asymptotic analysis of lattice Boltzmann algorithms including initial and boundary conditions. For the case of convection diffusion reaction equations, the analysis with this technique is carried out in [17] for a D1Q3 model, including a linear reaction $G(\rho)=-\kappa\rho$. In [23], results can be found for a D3Q17 multi-relaxation lattice Boltzmann model.

3.1 Formal analysis

The asymptotic analysis begins with the expansion of f_i:

$$f_i(n,j)=f_i^{(0)}(t_n,x_j)+hf_i^{(1)}(t_n,x_j)+h^2f_i^{(2)}(t_n,x_j)+\cdots, \tag{3.1}$$

where $f_i^{(k)}(t,x)$ are assumed to be sufficiently smooth functions in (t,x) and independent of h. Correspondingly,

$$\hat{\rho}=\rho_0+h\rho_1+h^2\rho_k+\cdots \tag{3.2}$$

with

$$\rho_k=\sum_{i=1}^{N}f_i^{(k)}. \tag{3.3}$$

Obviously ρ_k has at least the same smoothness as all $f_i^{(k)}$.

The expansion (3.1) is inserted into the lattice Boltzmann equations (2.3), (2.4) and Taylor expansion is applied to the terms $f_i^{(k)}(t_{n+1},x_j+hc_i)$ at (t_n,x_j), leading to

$$f_i^{(k)}(t_{n+1},x_j+hc_i)=f_i^{(k)}(t_n,x_j)+\sum_{m\geq 1}h^mD_i^mf_i^{(k)}(t_n,x_j). \tag{3.4}$$

Due to the diffusive scaling $\Delta t=h^2$, time and space derivatives mix in a particular way when the expansion is ordered in terms of powers of h. Eventually, this gives rise to the differential operators

$$D_i^m=\sum_{p+2q=m}\frac{1}{p!q!}\partial_t^q(c_i\partial_x)^p. \tag{3.5}$$

The expansion of $\hat{\rho}$ is further inserted into the reaction term g_i which leads to

$$g_i = g_i^{(0)} + h g_i^{(1)} + h^2 g_i^{(2)} + \cdots, \tag{3.6}$$

with $g_i^{(k)}(n,j) = -w_i \kappa(t_n,x_j)\rho_k(t_n,x_j)$.

Equating the terms in the same order of h, we obtain expressions for the expansion coefficients $f_i^{(k)}$ (where $A^\dagger$ is the pseudo-inverse of A),

$$\begin{aligned}
f_i^{(0)} &= w_i \rho_0,\\
f_i^{(1)} &= w_i(\rho_1 + \theta u c_i \rho_0) - \sum_{s=1}^{N} A_{is}^\dagger c_s \partial_x f_s^{(0)},\\
f_i^{(2)} &= w_i(\rho_2 + \theta u c_i \rho_1) - \sum_{s=1}^{N} A_{is}^\dagger \left\{ c_s \partial_x f_s^{(1)} + \left[\partial_t + \frac{1}{2}(c_s\partial_x)^2\right] f_s^{(0)} - g_i^{(0)} \right\},\\
f_i^{(3)} &= w_i(\rho_3 + \theta u c_i \rho_2)\\
&\quad - \sum_{s=1}^{N} A_{is}^\dagger \left\{ c_s \partial_x f_s^{(2)} + \left[\partial_t + \frac{1}{2}(c_s\partial_x)^2\right] f_s^{(1)} + \left[\partial_t c_s \partial_x + \frac{1}{6}(c_s\partial_x)^3\right] f_s^{(0)} - g_i^{(1)} \right\},\\
&\cdots
\end{aligned} \tag{3.7}$$

provided the moments ρ_k are solutions of certain partial differential equations which appear as solvability conditions in the derivation of the expansion coefficients. It turns out that ρ_0 has to satisfy the convection diffusion reaction equation (2.1) with

$$\nu = 2w_2\left(\frac{1}{\gamma_2} - \frac{1}{2}\right) \tag{3.8}$$

while ρ_1 is governed by a convection diffusion equation (2.1) with a linear reaction term,

$$\partial_t \rho_1 + \partial_x(u\rho_1) = \nu \partial_x^2 \rho_1 - \kappa \rho_1. \tag{3.9}$$

In particular, ρ_1 vanishes if zero initial values are assumed because the equation is homogeneous. Going further, the equation of ρ_2 is

$$\partial_t \rho_2 + \partial_x(u\rho_2) = \nu \partial_x^2 \rho_2 - \kappa \rho_2 + S(\rho_0) \tag{3.10}$$

with a source term $S(\rho_0)$ which involves various derivatives of ρ_0 that do not vanish in general. Therefore, ρ_2 will not disappear even with zero initial values. As an immediate consequence, the total density computed from the lattice Boltzmann result

$$\hat{\rho} = \rho_0 + h\rho_1 + h^2\rho_2 + \cdots$$

is the sum of the desired solution ρ_0 and additional, unwanted contributions like $h\rho_1$ or $h^2\rho_2$. Even if $\rho_1 = 0$, which usually can be achieved by using proper initial conditions, the contribution $h^2\rho_2$ will be the leading order of the numerical error so that the accuracy of the lattice Boltzmann scheme (2.3), (2.4) is restricted to second order in h.

3.2 Analysis of initial condition

A simple initial condition for f_i is the equilibrium function computed with the initial density ϕ,

$$f_i(0,j) = F_i^{eq}(\phi). \tag{3.11}$$

Inserting the expansion of f_i, we obtain

$$\begin{aligned} f_i^{(0)}(0,j) &= w_i\phi, \\ f_i^{(1)}(0,j) &= w_i\theta\phi u c_i, \\ f_i^{(k)}(0,j) &= 0, \quad k \geq 2. \end{aligned} \tag{3.12}$$

This result is compatible in leading order with the expressions in (3.7), provided

$$\rho_0(0,j) = \phi. \tag{3.13}$$

In first order, however, the condition can only be satisfied together with (3.7) if, initially, $\rho_1 = 0$ and ρ_0 is constant in space. Otherwise, the space derivative of $f^{(0)}$ does not vanish, and the two conditions together contradict the original smoothness assumption on the first order coefficient. In other words, the simple initialization (3.11) is incompatible with a smooth description of the numerical results up to first order in h.

One can cure this problem by modifying (3.11). The idea is simply to incorporate those terms from (3.7) into the initial condition which are missing in first order. Then, non-smooth behavior appears only at second order. Explicitly, the condition has the form

$$f_i(0,j) = F_i^{eq}(\phi) - h\sum_{s=1}^{N} A_{is}^{\dagger} w_s c_s \partial_x \phi. \tag{3.14}$$

3.3 A representation of f_i

The discussion in the previous section suggests a splitting of the lattice Boltzmann solution into a smooth and a non-smooth part $\tilde{f}_i$

$$f_i(n,j) = \bar{f}_i^{(0)}(t_n,x_j) + \cdots + h^k \bar{f}_i^{(K)}(t_n,x_j) + h^{K-1}\tilde{f}_i(n,j). \tag{3.15}$$

This idea can be traced back to the study of the Navier-Stokes and Euler limits in case of the continuous Boltzmann equation [4,15]. The structural form of the smooth coefficients $\bar{f}_i^{(k)}$ originates from (3.7) by replacing ρ_0 with the solution ρ of (2.1) and $\rho_k = 0$ for all $k \geq 1$.

$$\begin{aligned} \bar{f}_i^{(0)} &= w_i\rho, \\ \bar{f}_i^{(1)} &= w_i\theta u c_i \rho - \sum_{s=1}^{N} A_{is}^{\dagger} c_s \partial_x \bar{f}_s^{(0)}, \end{aligned}$$

$$\bar{f}_i^{(2)} = -\sum_{s=1}^{N} A_{is}^{\dagger}\left\{c_s\partial_x\bar{f}_s^{(1)} + \left[\partial_t + \frac{1}{2}(c_s\partial_x)^2\right]\bar{f}_s^{(0)} + w_s\kappa\rho\right\},$$
$$\bar{f}_i^{(3)} = -\sum_{s=1}^{N} A_{is}^{\dagger}\left\{c_s\partial_x\bar{f}_s^{(2)} + \left[\partial_t + \frac{1}{2}(c_s\partial_x)^2\right]\bar{f}_s^{(1)} + \left[\partial_t c_s\partial_x + \frac{1}{6}(c_s\partial_x)^3\right]\bar{f}_s^{(0)}\right\}. \tag{3.16}$$

Obviously, these coefficients depend solely on ρ and the data of the problem. If the scheme is used with the simple initialization (3.11), smoothly expanding up to $K=2$ is a reasonable choice in (3.15) because non-smooth behavior is expected already in first order. For the improved algorithm (3.14), the initial non-smooth behavior is pushed to second order, so that $K=3$ is reasonable.

For $K\leq 3$, the smooth part is constructed in such a way that its total density is the solution ρ of (2.1). Hence, we get the following relationship to the numerical value $\hat{\rho}$

$$\hat{\rho} = \rho + h^{K-1}\tilde{\rho}, \quad \text{with} \quad \tilde{\rho} = \sum_{i=1}^{N}\tilde{f}_i. \tag{3.17}$$

If we can show that $\tilde{\rho}$ is bounded independent of h, then h^{K-1} is the convergence order of the lattice Boltzmann method which is first order for initialization (3.11) and second order for (3.14).

To achieve this goal, we will deduce a bound on $\tilde{f}_i$. The basis for this estimate is the equation satisfied by $\tilde{f}_i$ which can be shown to be similar to the original lattice Boltzmann equation (2.3), (2.4) because both are linear and the smooth part satisfies them up to a small residue.

$$\tilde{f}_i(n+1, j+c_i) = \tilde{f}_i^{(c)}(n,j), \tag{3.18}$$

with

$$\tilde{f}_i^{(c)}(n,j) = \tilde{f}_i(n,j) + J_i(\tilde{\boldsymbol{f}}(n,j)) + h^2\tilde{g}_i(n,j) + h^2 R_i(n,j). \tag{3.19}$$

Here, $\boldsymbol{R}$ collects remainder terms resulting from the application of Taylor's theorem to the smooth part of the solution

$$R_i(n,j) = \sum_{s=0}^{K} D_i^{K+1-s}\bar{f}_i^{(s)}(t_{nis}, x_{jis}), \tag{3.20}$$

where t_{nis}, x_{jis} are certain points intermediate to the grid nodes. The reaction term has the form

$$\tilde{g}_i(n,j) = -w_i\kappa(t_n, x_j)\tilde{\rho}(n,j). \tag{3.21}$$

4 Stability analysis

A rigorous stability result of lattice Boltzmann methods with linear collision for Stokes flows has been presented in [14], with which not only the convergence of linear lattice

Boltzmann methods for Stokes flows but also nonlinear ones for Navier-Stokes flows are proved. Here, we extend the idea to the lattice Boltzmann method for the convection-diffusion-reaction equation.

In order to formulate the stability conditions and to perform the convergence analysis, it is useful to reformulate the original algorithm in operator notation.

4.1 The lattice Boltzmann equation in operator notation

The collision phase of the lattice Boltzmann algorithm works locally. Due to the linearity of the equilibrium function, we can write

$$\boldsymbol{f}^{eq} = E\boldsymbol{f}, \quad \boldsymbol{f}^{(c)} = C\boldsymbol{f}, \tag{4.1}$$

with suitable matrices E and C. Moreover, we would like to split E into a constant part and a generally nonconstant part depending on the convection speed, i.e. $E = E^0 + hE^u$. Their matrix representations for D1Q2 and D1Q3 models are given as follows:

D1Q2:

$$E^0 = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad E^u = \theta\frac{u}{2}\begin{pmatrix} -1 & -1 \\ 1 & 1 \end{pmatrix}. \tag{4.2}$$

D1Q3:

$$E^0 = \begin{pmatrix} 1-2b & 1-2b & 1-2b \\ b & b & b \\ b & b & b \end{pmatrix}, \quad E^u = \theta u \begin{pmatrix} 0 & 0 & 0 \\ -b & -b & -b \\ b & b & b \end{pmatrix}. \tag{4.3}$$

Accordingly we have a collusion operator $C = I + J$ with $J = J^0 + hJ^u$ which have the matrix forms,

$$J^0 = A(E^0 - I), \quad J^u = AE^u. \tag{4.4}$$

The transport phase describes the particle movement to the neighboring nodes and is expressed with a non-local operator S as introduced in [11, 12, 14]. Considering the block-vector $\boldsymbol{f}(n)$ which contains $\boldsymbol{f}(n,j)$ in its jth block, the action of S on $\boldsymbol{f}(n)$ is merely a permutation, because transport just moves components $f_i(n,j)$ from block j into corresponding components of the neighboring blocks (in case of non-periodic boundary conditions like the bounce back rule, it is also possible that the component number i is changed during transport).

Interpreting the collision operators as block-diagonal matrices when acting on the block-vector $\boldsymbol{f}(n)$, we finally obtain the compact form of our lattice Boltzmann scheme

$$S\boldsymbol{f}(n+1) = C\boldsymbol{f}(n) + h^2\boldsymbol{g}(n), \tag{4.5}$$

or with expanded collision operator

$$S\boldsymbol{f}(n+1) = (I + J^0 + hJ^u)\boldsymbol{f}(n) + h^2\boldsymbol{g}(n). \tag{4.6}$$

Similarly, the equation for $\tilde{\boldsymbol{f}}$ can be cast into the form

$$S\tilde{\boldsymbol{f}}(n+1)=(I+J^0+hJ^u)\tilde{\boldsymbol{f}}(n)+h^2\tilde{\boldsymbol{g}}(n)+h^2\boldsymbol{R}(n). \tag{4.7}$$

In order to estimate vectors and block-vectors as well as related operators, we introduce a weighted inner product for vectors in $\mathbb{R}^N$ with associated norm (see [14]) using positive weighs $a_i>0$

$$\langle \boldsymbol{f},\boldsymbol{g}\rangle_a=\sum_{i=1}^N a_i f_i g_i, \quad \forall \boldsymbol{f},\boldsymbol{g}\in\mathbb{R}^N, \tag{4.8}$$

$$\|\boldsymbol{f}\|_a^2=\sum_{i=1}^N a_i f_i^2=\|P\boldsymbol{f}\|^2. \tag{4.9}$$

Here, the norm without index refers to the unweighed case which amounts to $a_i=1$ for all i.

For grid functions from $V_h=\{\boldsymbol{f}\mid \boldsymbol{f}(j)\in\mathbb{R}^N, \forall x_j\in\Omega\}$ like the lattice Boltzmann solution (here Ω is a periodicity cell), the L_2 norm and a-norm in 1D are given as follows,

$$\|\boldsymbol{f}\|_\Omega^2=\sum_{x_j\in\Omega} h\|\boldsymbol{f}(j)\|^2, \quad \|\boldsymbol{f}\|_{a,\Omega}^2=\sum_{x_j\in\Omega} h\|\boldsymbol{f}(j)\|_a^2, \tag{4.10}$$

and the associated operator norms are

$$\|C\|_a=\sup_{x\in\mathbb{R}^N\setminus\{0\}}\frac{\|Cx\|_a}{\|x\|_a}, \quad \|B\|_{a,\Omega}=\sup_{x\in V_h\setminus\{0\}}\frac{\|Bx\|_{a,\Omega}}{\|x\|_{a,\Omega}}. \tag{4.11}$$

4.2 The stability structure

A crucial ingredient for stability estimates of lattice Boltzmann algorithms is the stability structure $(P,\boldsymbol{a},\boldsymbol{\lambda})$, which is first proposed in [1] and later extended in [14]. Here, $P\in\mathbb{R}^{N\times N}$ collects all the left eigenvectors of the collision operator J corresponding to the eigenvalues $-\lambda_i$. Stability is obtained under the condition

$$\lambda_i\in[0,2], \quad PJ=-\mathrm{diag}(\boldsymbol{\lambda})J, \quad P^TP=\mathrm{diag}(\boldsymbol{a}). \tag{4.12}$$

As stated in [14], $a_i>0$ is guaranteed and can be used to define weighted norms as introduced in the previous section.

The procedure to find a stability structure for some specific collision matrix J consists of the following steps: First, we compute the eigenvalues and left eigenvectors of J. This is generally possible even for large velocity sets because the eigenstructure of the relaxation matrix is known by construction and the eigenvectors are closely related to the equilibrium function. After that step, the rows of P are determined up to certain non-zero factors. In the second step, one tries to fix these constants in such a way that the remaining condition $P^{\mathsf{T}}P=\mathrm{diag}(\boldsymbol{a})$ is satisfied.

To illustrate this crucial computation in the case of the D1Q2 model with pure diffusion, we start with the related collision matrix

$$J^0 = \frac{\gamma_2}{2}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{4.13}$$

Here eigenvectors are easily spotted as

$$\boldsymbol{p}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \boldsymbol{p}_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

with corresponding negative eigenvalues $\lambda_1 = 0$ and $\lambda_2 = \gamma_2$. Inserting general multiples of $\boldsymbol{p}_1$ and $\boldsymbol{p}_2$ into the rows of a matrix Q leads to

$$Q = \begin{pmatrix} \alpha & \alpha \\ -\beta & \beta \end{pmatrix}$$

and computing the product Q^TQ results in

$$Q^TQ = \begin{pmatrix} \alpha & -\beta \\ \alpha & \beta \end{pmatrix}\begin{pmatrix} \alpha & \alpha \\ -\beta & \beta \end{pmatrix} = \begin{pmatrix} \alpha^2+\beta^2 & \alpha^2-\beta^2 \\ \alpha^2-\beta^2 & \alpha^2+\beta^2 \end{pmatrix}.$$

As a consequence, we see that a diagonal matrix with positive diagonals is achieved if $|\alpha| = |\beta| \neq 0$, for example $\alpha = \beta = 1$, i.e.

$$P = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}.$$

Along these lines, we obtain the following result for the collision operator J^0 in case of pure diffusion and also in a case with constant convection and reaction coefficients presented below. The proof of these results amounts to checking the somewhat tedious but straight forward computations which are hidden.

Theorem 4.1. *In the D1Q2 and D1Q3 lattice Boltzmann schemes with $\gamma_i \in [0,2]$ for $i \geq 2$, the collision operator J^0 admits a stability structure $(P, \boldsymbol{a}, \boldsymbol{\lambda})$, so that on periodic domains*

$$\|S\|_{a,\Omega} = 1, \quad \|I + J^0\|_a \leq 1, \quad \|I + J^0\|_{a,\Omega} \leq 1. \tag{4.14}$$

A stability structure for the D1Q2 model is

$$P = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} 2 \\ 2 \end{pmatrix}, \quad \boldsymbol{\lambda} = \begin{pmatrix} 0 \\ \gamma_2 \end{pmatrix}; \tag{4.15}$$

and for the D1Q3 model

$$P = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -\frac{1}{\sqrt{2b}} & \frac{1}{\sqrt{2b}} \\ -\sqrt{\frac{2b}{1-2b}} & \sqrt{\frac{1-2b}{2b}} & \sqrt{\frac{1-2b}{2b}} \end{pmatrix}, \quad \boldsymbol{a} = \begin{pmatrix} \frac{1}{1-2b} \\ \frac{1}{b} \\ \frac{1}{b} \end{pmatrix}, \quad \boldsymbol{\lambda} = \begin{pmatrix} 0 \\ \gamma_2 \\ \gamma_3 \end{pmatrix}. \tag{4.16}$$

In both cases, the weight vector $\boldsymbol{a}$ contains the inverse weights $1/w_i$ of the corresponding model.

Proof. In the D1Q2 case, J^0 is given by (4.13) so that $PJ^0 = -\mathrm{diag}(\boldsymbol{\lambda})P$ is easily checked. Similarly, the computation of $P^{\mathsf{T}}P = \mathrm{diag}(2,2)$ is straight forward. In the D1Q3 case, we have

$$J^0 = \frac{\gamma_2}{2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & -1 \end{pmatrix} + \frac{\gamma_3}{2}\begin{pmatrix} -4b & -2(2b-1) & -2(2b-1) \\ 2b & 2b-1 & 2b-1 \\ 2b & 2b-1 & 2b-1 \end{pmatrix} \tag{4.17}$$

and the stability conditions are again easily checked.

Since $0 \le \lambda_i \le 2$, we have $|1-\lambda_i| \le 1$. Thus for any $\boldsymbol{f} \in \mathbb{R}^N$ holds

$$\left\|(I+J^0)\boldsymbol{f}\right\|_a = \left\|P(I+J^0)\boldsymbol{f}\right\|^2 = \|(I-\mathrm{diag}(\lambda))P\boldsymbol{f}\|^2 \le \|P\boldsymbol{f}\|^2 = \|\boldsymbol{f}\|_a^2. \tag{4.18}$$

Finally, the isometry property of S follows from a direct application of Lemma 1 in [14] to the 1D case. □

Obviously, for the whole collision operator $J = J^0 + hJ^u$ one cannot expect a stability structure in general, since the convection speed u is a function of (t,x). However, for the special case of constant convection speed and constant reaction coefficient, a stability structure can be derived, at least for the BGK-case where all eigenvalues γ_i of the relaxation matrix are identical.

Theorem 4.2. *Assume that the convection u and the reaction rate κ are constant and both D1Q2 and D1Q3 lattice Boltzmann schemes are based on the BGK collision model $J = \frac{1}{\tau}(E^0 + hE^u - I)$. Then for all $\tau \ge 1/2$ and all h constrained by*

$$0 < \beta = 1 - \tau\kappa h^2 \le 1, \quad \theta|u|h < \beta, \tag{4.19}$$

$J + h^2 J^\kappa$ with $J^\kappa = -\kappa E^0$ admits a stability structure $(P_h, \boldsymbol{a}_h, \boldsymbol{\lambda}_h)$. Based on this structure, we find again

$$\|S\|_{a_h,\Omega} = 1, \quad \left\|I + J + h^2 J^\kappa\right\|_{a_h,\Omega} \le 1. \tag{4.20}$$

The stability structure for the D1Q2 model is

$$P_h = \begin{pmatrix} 1 & 1 \\ -\sqrt{\frac{\beta+\theta uh}{\beta-\theta uh}} & \sqrt{\frac{\beta-\theta uh}{\beta+\theta uh}} \end{pmatrix}, \quad \boldsymbol{a}_h = 2\beta\begin{pmatrix} \frac{1}{\beta-\theta uh} \\ \frac{1}{\beta+\theta uh} \end{pmatrix}, \quad \boldsymbol{\lambda}_h = \begin{pmatrix} \kappa h^2 \\ \frac{1}{\tau} \end{pmatrix}; \tag{4.21}$$

and for the D1Q3 model

$$P_h = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -\sqrt{\frac{\beta+\theta uh}{2b(\beta-\theta uh)}} & \sqrt{\frac{\beta-\theta uh}{2b(\beta+\theta uh)}} \\ -\sqrt{\frac{2b}{1-2b}} & \sqrt{\frac{1-2b}{2b}} & \sqrt{\frac{1-2b}{2b}} \end{pmatrix}, \quad \boldsymbol{a}_h = \begin{pmatrix} \frac{1}{1-2b} \\ \frac{\beta}{b(\beta-\theta uh)} \\ \frac{\beta}{b(\beta+\theta uh)} \end{pmatrix}, \quad \boldsymbol{\lambda}_h = \begin{pmatrix} \kappa h^2 \\ \frac{1}{\tau} \\ \frac{1}{\tau} \end{pmatrix}. \tag{4.22}$$

While the proof is essentially a copy of the one in Theorem 4.1, the underlying derivation of the stability structure is more involved due to the much richer structure of the collision operator $J^0+hJ^u+h^2J^\kappa$.

To illustrate the result in more detail, we begin with a discussion of the stability conditions. First of all, it is clear that the condition $\gamma_i\in[0,2]$ known from Theorem 4.1 must reappear because $u=\kappa=0$ is a valid choice of parameters. Since, for BGK models, $\gamma_1=\gamma_2=1/\tau$ we find this condition in the form $\tau\geq 1/2$.

Since the availability of a stability structure entails that the lattice Boltzmann evolution operator is bounded by 1 in a suitable norm, we anticipate that cases with systematically growing solutions are excluded. Keeping in mind that the equation in our framework reads

$$\partial_t\rho+\partial_x(u\rho)=\nu\partial_x^2\rho-\kappa\rho,$$

such solutions would arise if the reaction coefficient κ was negative and, indeed, the condition $\beta=1-\tau\kappa h^2\leq 1$ extracted from (4.19) forbids that by requiring $\kappa\geq 0$.

While this is a structural condition on the data, the remaining two conditions encoded in (4.19) lead to restrictions on space step $\Delta x=h$ and time step $\Delta t=h^2$. For example, $0<\beta$ amounts to $\Delta t<1/(\tau\kappa)$ which is a typical stability condition for explicit time discretizations schemes applied to equations with source terms.

Finally, the condition $\theta|u|h<\beta$ is related to convection and has the typical form of a CFL condition $|u|\Delta t/\Delta x<C$ with the CFL number $C=\beta/\theta$.

While (4.19) has to be observed for any specific choice of u,κ,τ,θ and h, we note that for fixed data but $h\to 0$ it will eventually be satisfied as long as $\kappa\geq 0$.

We conclude this section with a technical remark. Compared to previous applications of the stability structure in [11, 12], a new feature is the h-dependency of the collision matrix which leads to h-depending ingredients of the stability structure and, as a consequence, also of the induced norms. However, one can easily see that $P_h\to P$, $\boldsymbol{a}_h\to\boldsymbol{a}$ and $\boldsymbol{\lambda}_h\to\boldsymbol{\lambda}$ in the limit of $h\to 0$ where the limits are the corresponding values from Theorem 4.1. In particular, the convergence proofs presented in the next section are only mildly influenced by this technicality.

5 Convergence results

In this section, ρ always refers to the solution of (2.1) and we assume enough smoothness so that all expansion arguments required in the asymptotic analysis can be carried out. More specifically, we require

$$\rho\in C^{K+1}([0,T]\times\mathbb{R}),\quad u\in C^K([0,T]\times\mathbb{R}),\quad \kappa\in C^{K-1}([0,T]\times\mathbb{R}). \tag{5.1}$$

Here the choice of $K\leq 3$ depends on the chosen initial condition. We assume $K>K_0$ where $K_0=1$ for the simple initialization (3.11) and $K_0=2$ in case (3.14).

Our first result ensures a bound for the non-smooth part of the lattice Boltzmann solution.

Theorem 5.1. *Under the general assumptions of this section, there exist h-independent constants C_0 and C_R such that*

$$\|\tilde{\boldsymbol{f}}(0)\|_{a,\Omega} \leq h^{1-K+K_0} C_0 \max(\boldsymbol{a}), \quad \|\boldsymbol{R}\|_{a,\Omega} \leq C_R \max(\boldsymbol{a}). \tag{5.2}$$

Proof. The proof is straightforward. The regularity of ρ, u and κ yields $|R_i(n,j)| = \mathcal{O}(1)$. Thus there is a constant c_R such that $\|\boldsymbol{R}(n,j)\|_a \leq c_R \max(\boldsymbol{a})$. After summing over the domain, we find

$$\|\boldsymbol{R}(n,j)\|_{a,\Omega} \leq c_R \max(\boldsymbol{a}) \sqrt{\sum_{x_j \in \Omega} h} = C_R \max(\boldsymbol{a}).$$

On the other hand,

$$\tilde{f}_i(0,j) = h^{1-K} \left[f_i(0,j) - \sum_{s=0}^{K} h^\kappa \bar{f}_i^{(s)}(0,x_j) \right] = h^{1-K+K_0} \sum_{s=K_0}^{K} h^{s-K_0} \bar{f}_i^{(s)}(0,x_j). \tag{5.3}$$

Again the sum on the right hand side is bounded due to the regularity of ρ, u and κ. $\square$

In case that the weight a is deduced from the stability structure in Theorem 4.1, $\max(\boldsymbol{a})$ is constant, whereas in Theorem 4.2 $\max(\boldsymbol{a}_h)$ is h-dependent. However, the h-dependence does not change any order because the limit of $\max(\boldsymbol{a}_h)$ is $\max(\boldsymbol{a})$ as $h \to 0$.

5.1 Constant coefficient cases

In order to illustrate how the availability of a stability structure can be used directly to ensure convergence, we consider the case of constant coefficients u,κ which is related to the situation in Theorem 4.2. Since this result has been derived for the BGK collision model only, we work with a single relaxation time τ for this illustration. However, in the special case $u = \kappa = 0$ we could switch to Theorem 4.1 which ensures the crucial stability structure also for more general collision models.

Theorem 5.2. *Assume, apart from the general assumptions of this section, that u,κ are constant with $\kappa \geq 0$ and let all eigenvalues γ_i be equal to $1/\tau \leq 2$. Then there exists $h_0 > 0$ such that for all $0 < h \leq h_0$ the solution of the lattice Boltzmann scheme* (2.4), (2.3) *with BGK model has a non-smooth part which satisfies*

$$\|\tilde{\boldsymbol{f}}(n)\|_{a,\Omega} \leq \|\tilde{\boldsymbol{f}}(0)\|_{a,\Omega} + T C_R \max(\boldsymbol{a}_h), \quad \forall n h^2 \leq T \tag{5.4}$$

and

$$\|\hat{\rho}(n) - \rho(t_n)\| \leq C h^{K_0}, \quad \forall n h^2 \leq T. \tag{5.5}$$

Proof. If $\tau \geq 1/2$ and $\kappa \geq 0$, the conditions (4.19) in Theorem 4.2 are satisfied for sufficiently small h. Moreover, the equation for $\tilde{\boldsymbol{f}}$ has the form

$$S\tilde{\boldsymbol{f}}(n+1) = (I + J + h^2 J^\kappa) \tilde{\boldsymbol{f}}(n) + h^2 \boldsymbol{R}(n) \tag{5.6}$$

with $J^\kappa = -\kappa E^0$. Using the stability result (4.20) we obtain

$$\begin{aligned}\|\tilde{\boldsymbol{f}}(n+1)\|_{a_h,\Omega} &\le \|(I+J^0+h^2J^\kappa)\tilde{\boldsymbol{f}}(n)\|_{a_h,\Omega}+h^2\|\boldsymbol{R}(n)\|_{a_h,\Omega}\\ &\le \|\tilde{\boldsymbol{f}}(n)\|_{a_h,\Omega}+h^2\|\boldsymbol{R}(n)\|_{a_h,\Omega}. \end{aligned}\tag{5.7}$$

Applying this inequality recursively leads to

$$\|\tilde{\boldsymbol{f}}(n+1)\|_{a_h,\Omega} \le \|\tilde{\boldsymbol{f}}(0)\|_{a_h,\Omega}+h^2\sum_{s=0}^{n}\|\boldsymbol{R}(s)\|_{a_h,\Omega}. \tag{5.8}$$

Finally, applying the results of Theorem 5.1, we obtain for all n with $nh^2 \le T$

$$\|\tilde{\boldsymbol{f}}(n+1)\|_{a_h,\Omega} \le \|\tilde{\boldsymbol{f}}(0)\|_{a_h,\Omega}+TC_R\max(\boldsymbol{a}_h). \tag{5.9}$$

Since $\hat{\rho}(n,j)=\rho(t_n,x_j)+h^{K-1}\sum_{i=1}^N \tilde{f}_i(n,j)$ and the summation is actually the first entry of $P\tilde{\boldsymbol{f}}(n,j)$, it follows

$$\hat{\rho}(n,j)-\rho(t_n,x_j)=h^{K-1}(P\tilde{\boldsymbol{f}}(n,j))_1. \tag{5.10}$$

Noting that

$$(P\tilde{\boldsymbol{f}}(n,j))_1^2 \le (P\tilde{\boldsymbol{f}}(n,j))_1^2+\cdots+(P\tilde{\boldsymbol{f}}(n,j))_N^2=\|P\tilde{\boldsymbol{f}}(n,j)\|^2 \tag{5.11}$$

and taking L_2 norm on the whole domain leads to

$$\|\hat{\rho}(n)-\rho(t_n)\|_\Omega = h^{K-1}\|(P\tilde{\boldsymbol{f}}(n,j))_1\|_\Omega \le h^{K-1}\|P\tilde{\boldsymbol{f}}(n)\|_\Omega = h^{K-1}\|\tilde{\boldsymbol{f}}(n)\|_{a_h,\Omega}. \tag{5.12}$$

Taking into account (5.4) and the estimate (5.2) we finally get

$$\|\hat{\rho}(n)-\rho(t_n)\|_\Omega \le h^{K-1}[\|\tilde{\boldsymbol{f}}(0)\|_{a_h,\Omega}+TC_R\max(\boldsymbol{a}_h)] \le (h^{K_0}C_0+h^{K-1}TC_R)\max(\boldsymbol{a}_h). \tag{5.13}$$

Since $\boldsymbol{a}_h \to \boldsymbol{a}$ in the limit $h\to 0$, there exists $h_0>0$ so that for any $h\le h_0$ which also guarantees condition (4.19), we find $\max(\boldsymbol{a}_h)\le\max(\boldsymbol{a})+1$. □

5.2 Convergence in the general case

Finally, we consider the case where the data of the problem is space and time dependent. Now the strategy of the convergence proof has to be modified, because a direct construction of a stability structure is no longer possible. A detailed investigation in this case relies on properties of the constant part J^0 of the collision operator, the proof of which is presented in Appendix A.

Theorem 5.3. *Let the eigenvalues of the relaxation matrix satisfy $\gamma_i \in [0,2]$ for $i>1$. If the eigenvalue γ_2, which determines the diffusivity, satisfies $0<\gamma_2<2$ strictly, then*

$$\|I+J+h^2J^\kappa\|_{a,\Omega} \le \sqrt{1+\alpha h^2},$$

with $J^\kappa=-\kappa E^0$. Here $\alpha=\frac{\gamma_2}{2-\gamma_2}u_\infty^2\theta+2\kappa_\infty+h^2\kappa_\infty^2$ and u_∞ and κ_∞ represent the maximum norm of u and κ respectively. In the particular case $\kappa\ge 0$ and $h\le\sqrt{2/\kappa_\infty}$, we have $\alpha=\frac{\gamma_2}{2-\gamma_2}u_\infty^2\theta$.

Since the sign of κ is generally not restricted in this result, it is clear that the solution can grow exponentially in time. This is reflected by the operator norm estimate, which now yields a bound which is slightly larger than unity, so that controlled growth over many time steps is possible.

Theorem 5.4. *Under the general assumption of this section and the assumptions of Theorem* 5.3, *we find*

$$\|\tilde{\boldsymbol{f}}(n)\|_{a,\Omega} \leq \left[\|\tilde{\boldsymbol{f}}^0\|_{a,\Omega} + TC_R \max(\boldsymbol{a})\right]\sqrt{\exp(\alpha T)}, \tag{5.14}$$

$$\|\hat{\rho}(n) - \rho(t_n)\| \leq C\sqrt{\exp(T\alpha)}h^{K_0}, \quad \forall nh^2 \leq T. \tag{5.15}$$

Proof. Applying the result of Theorem 5.3 to the equation for $\tilde{\boldsymbol{f}}$, we achieve

$$\begin{aligned}\|\tilde{\boldsymbol{f}}(n+1)\|_{a,\Omega} &\leq \|(I+J+h^2J^\kappa)\tilde{\boldsymbol{f}}(n)\|_{a,\Omega} + h^2\|\boldsymbol{R}(n)\|_{a,\Omega} \\ &\leq \sqrt{1+\alpha h^2}\,\|\tilde{\boldsymbol{f}}(n)\|_{a,\Omega} + h^2\|\boldsymbol{R}(n)\|_{a,\Omega},\end{aligned} \tag{5.16}$$

Applying this inequality recursively with respect to n, we finally obtain

$$\begin{aligned}\|\tilde{\boldsymbol{f}}(n)\|_{a,\Omega} &\leq (1+\alpha h^2)^{\frac{n}{2}}\|\tilde{\boldsymbol{f}}(0)\|_{a,\Omega} + h^2\sum_{s=0}^{n-1}(1+\alpha h^2)^{\frac{n-s}{2}}\|\boldsymbol{R}(s)\|_{a,\Omega} \\ &\leq \sqrt{\exp(\alpha T)}\left[\|\tilde{\boldsymbol{f}}(0)\|_{a,\Omega} + TC_R\max(\boldsymbol{a})\right].\end{aligned} \tag{5.17}$$

From this, relation (5.15) is concluded as in the previous cases. □

Obviously, the estimate of the collision operator for the pure diffusion in Theorem 4.1 can be taken as a special case of Theorem 5.3, where $u=0$ and $\kappa=0$ lead to $\alpha=0$. Hence, the convergence result on periodic domains in [22] is included in the above theorem and the same strategy can be applied to the schemes in [7].

6 Conclusion

We have proved the convergence of standard one-dimensional lattice Boltzmann methods with collision operators including BGK and MRT models for a class of convection-diffusion-reaction equations on periodic domains. In all cases, convergence is of second order in the grid size but may be lower if suboptimal initialization procedures are used.

For constant convection speeds and reaction coefficients, it is possible to derive a stability structure in the case of BGK collision operators and, based on this, prove stability of the whole lattice Boltzmann evolution operator. Combined with the consistency result, convergence follows immediately.

The most general scenario with space and time dependent data and general MRT relaxation matrices requires a different strategy. Here, we use the stability structure of the constant part J^0 of the collision operator to derive a bound for the error terms of the approximation and finally get convergence.

With these two scenarios, our strategy to prove convergence is nicely illustrated. An extension to higher dimensional (2D and 3D) cases, nonlinear reaction terms, other boundary conditions, and also other equilibrium functions (see [11, 12]) is possible. For the convection-diffusion-reaction equation, corresponding results will be presented in subsequent papers.

A Proof of Theorem 5.3

In order to estimate the effect of the collision process, we need a few fundamental observations about the stability structure in the pure diffusion case.

Introducing the matrix $W_{ij}=a_i^{-1}\delta_{ij}$ with the inverse components of $\boldsymbol{a}$ on its diagonal, we first observe that $P^TP=\mathrm{diag}(\boldsymbol{a})$ implies (by multiplication with P^{-T} from the left and WP^T from the right)

$$PWP^T=I$$

which means that the rows r_i^T of P are orthonormal with respect to the weighted scalar product $(x,y)\mapsto x^TWy$. Introducing the matrices

$$P_i=W^{\frac{1}{2}}r_ir_i^T,\quad i=1,\cdots,N,$$

we can use the fact that r_i is a left eigenvector of J^0 to show that

$$P_iJ^0=W^{\frac{1}{2}}r_i(-\lambda_i)r_i^T=-\lambda_iP_i.$$

Moreover, the orthogonality relation yields

$$P_i^TP_j=r_i(r_i^TWr_j)r_j^T=r_ir_i^T\delta_{ij},\quad i,j=1,\cdots,N,$$

and hence

$$P^TP=\sum_{i=1}^N r_ir_i^T=\sum_{i=1}^N P_i^TP_i, \tag{A.1}$$

as well as

$$\|P_i\boldsymbol{g}\|=\left\langle P_i^TP_i\boldsymbol{g},\boldsymbol{g}\right\rangle^{\frac{1}{2}}=\left\langle r_ir_i^T\boldsymbol{g},\boldsymbol{g}\right\rangle^{\frac{1}{2}}=|r_i^T\boldsymbol{g}|=|(P\boldsymbol{g})_i|.$$

Altogether, we have

Lemma A.1. *Let r_m^T $(m=1,\cdots,N)$ be the row vectors of the matrix P in the stability structure of J^0 and $W=\mathrm{diag}(1/a_1,\cdots,1/a_N)$. Then*

$$P^TP=\sum_{m=1}^N P_m^TP_m,\quad P_m=W^{\frac{1}{2}}r_mr_m^T, \tag{A.2}$$

and P_m possess the following properties

$$\begin{aligned}&(i)\ P_i^T P_m = \delta_{im} P_m^T P_m, \quad P_m J^0 = -\lambda_m P_m;\\&(ii)\ P_1 J^0 = 0;\\&(iii)\ P_m J^u = \delta_{m2}\lambda_2 u\sqrt{\theta} W^{\frac{1}{2}} r_2 r_1^T, \quad \forall m = 1,\cdots,N;\\&(iv)\ P_m J^\kappa = -\delta_{m1}\kappa P_1, \quad \forall m = 1,\cdots,N.\end{aligned} \tag{A.3}$$

We note that

$$\|P_m \boldsymbol{g}\| = \left\| W^{\frac{1}{2}} r_m r_m^T \boldsymbol{g} \right\| = |r_m^T \boldsymbol{g}| = |(P\boldsymbol{g})_m|, \quad \forall m = 1,\cdots,N. \tag{A.4}$$

Proof. The statements (A.2) and (i) have already been shown above and (ii) is a special case of (i) with $\lambda_1 = 0$. By direct checking, we see that the row vectors r_m^T are the left eigenvectors not only of J^0 but also of A as well as E^0. In fact, $r_m^T A = \lambda_k r_m^T$, $r_m^T E^0 = \delta_{m1} r_m^T$. Immediately we have $P_m J^\kappa = -\kappa P_m E^0 = -\delta_{m1}\kappa P_1$.

On the other hand, $r_m^T E^u = \delta_{m2} u\sqrt{\theta} r_1^T$. Therefore, $P_1 J^u = W^{\frac{1}{2}} r_1 r_1^T A E^u = \lambda_1 W^{\frac{1}{2}} r_1 r_1^T E^u = 0$. For the D1Q3 model, it also holds $P_3 J^u = 0$. □

To estimate the norm of the full collision operator, we begin with an investigation of $\left\|(I+J+h^2 J^\kappa)\boldsymbol{g}\right\|_a^2$ for some arbitrary $\boldsymbol{g} \in \mathbb{R}^N$. The expression is separated into several parts as follows

$$\left\|(I+J+h^2 J^\kappa)\boldsymbol{g}\right\|_a^2 = \|\boldsymbol{g}\|_a^2 + \sigma_1 + \sigma_2 + \sigma_3 + h^4 \|J^\kappa \boldsymbol{g}\|_a^2 \tag{A.5}$$

with

$$\begin{aligned}\sigma_1 &= h^2 \|J^u \boldsymbol{g}\|_a^2,\\ \sigma_2 &= \left\|J^0 \boldsymbol{g}\right\|_a^2 + 2\left\langle P^T P \boldsymbol{g}, J^0 \boldsymbol{g}\right\rangle + 2h\left\langle P^T P(I+J^0)\boldsymbol{g}, J^u \boldsymbol{g}\right\rangle,\\ \sigma_3 &= 2h^2\left\langle P^T P(I+J^0+hJ^u)\boldsymbol{g}, J^\kappa \boldsymbol{g}\right\rangle.\end{aligned} \tag{A.6}$$

With the results from Lemma A.1 (property (iii) in particular), it follows immediately

Lemma A.2. $\sigma_1 = h^2 \lambda_2^2 u^2 \theta \|P_1 \boldsymbol{g}\|^2$.

The diffusive nature of the collision process which follows from the strict inequalities in the assumption $0 < \lambda_2 < 2$ allows us to estimate σ_2 proportional to h^2.

Lemma A.3. $\sigma_2 \le h^2 (1-\lambda_2)^2 \frac{\lambda_2}{2-\lambda_2} u^2 \theta \|P_1 \boldsymbol{g}\|^2$.

Proof. Applying property (i) of Lemma A.1 we have

$$\Delta_1 = \left\|J^0 \boldsymbol{g}\right\|_a^2 = \left\langle P^T P J^0 \boldsymbol{g}, J^0 \boldsymbol{g}\right\rangle = \sum_{m=2}^{N} \lambda_m^2 \|P_m \boldsymbol{g}\|^2 \tag{A.7}$$

in which $\lambda_1 = 0$ has been inserted. Similarly

$$\Delta_2 = 2\left\langle P^T P\boldsymbol{g}, J^0\boldsymbol{g}\right\rangle = \sum_{m=2}^{N} (-2\lambda_m)\,\|P_m\boldsymbol{g}\|^2, \tag{A.8}$$

and

$$\Delta_3 = 2h\left\langle P^T P(I+J^0)\boldsymbol{g}, J^u\boldsymbol{g}\right\rangle = 2h\sum_{m=1}^{N}(1-\lambda_m)\left\langle P_m^T P_m\boldsymbol{g}, J^u\boldsymbol{g}\right\rangle = 2h(1-\lambda_2)\langle P_2\boldsymbol{g},\, P_2 J^u\boldsymbol{g}\rangle. \tag{A.9}$$

Substituting property (iii) renders

$$\begin{aligned}
\Delta_3 &= 2h(1-\lambda_2)\left\langle P_2\boldsymbol{g},\, \lambda_2 u\sqrt{\theta}W^{\frac{1}{2}} r_2 r_1^T\boldsymbol{g}\right\rangle = 2h(1-\lambda_2)\lambda_2 u\sqrt{\theta}\tilde{\rho}\left\langle P_2\boldsymbol{g},\, W^{\frac{1}{2}} r_2\right\rangle \\
&\le (2\lambda_2-\lambda_2^2)\,\|P_2\boldsymbol{g}\|^2 + h^2\frac{(1-\lambda_2)^2\lambda_2^2}{2\lambda_2-\lambda_2^2}u^2\theta\tilde{\rho}^2 \\
&\le (2\lambda_2-\lambda_2^2)\,\|P_2\boldsymbol{g}\|^2 + h^2(1-\lambda_2)^2\frac{\lambda_2}{2-\lambda_2}u^2\theta\,\|P_1\boldsymbol{g}\|^2.
\end{aligned} \tag{A.10}$$

In summary,

$$\begin{aligned}
\sigma_2 &= \Delta_1+\Delta_2+\Delta_3 \le \sum_{m>2}^{N}(\lambda_m^2-2\lambda_m)\,\|P_m\boldsymbol{g}\|^2 + h^2(1-\lambda_2)^2\frac{\lambda_2}{2-\lambda_2}u^2\theta\,\|P_1\boldsymbol{g}\|^2 \\
&\le h^2(1-\lambda_2)^2\frac{\lambda_2}{2-\lambda_2}u^2\theta\,\|P_1\boldsymbol{g}\|^2.
\end{aligned} \tag{A.11}$$

Obviously, $\sigma_2 \le 0$ in case that $\lambda_2 = 1$. □

Lemma A.4. $\sigma_3 = -2h^2\kappa\,\|P_1\boldsymbol{g}\|^2$.

Proof.

$$\begin{aligned}
\sigma_3 &= 2h^2\left\langle (I+J^0+hJ^u)\boldsymbol{g}, P^T P J^\kappa\boldsymbol{g}\right\rangle = 2h^2\sum_{m=1}^{N}\left\langle (I+J^0+hJ^u)\boldsymbol{g}, P_m^T P_m J^\kappa\boldsymbol{g}\right\rangle \\
&= 2h^2\left\langle (I+J^0+hJ^u)\boldsymbol{g}, P_1^T P_1 J^\kappa\boldsymbol{g}\right\rangle = 2h^2\langle P_1(I+J^0+hJ^u)\boldsymbol{g}, P_1 J^\kappa\boldsymbol{g}\rangle \\
&= 2h^2\langle P_1\boldsymbol{g}, -\kappa P_1\boldsymbol{g}\rangle = -2h^2\kappa\,\|P_1\boldsymbol{g}\|^2.
\end{aligned} \tag{A.12}$$

The proof is complete. □

With the help of the lemmas above, we can now finish the proof of Theorem 5.3.

$$\|J^\kappa\boldsymbol{g}\|_a^2 = \|PJ^\kappa\boldsymbol{g}\|^2 = \|P_1 J^\kappa\boldsymbol{g}\|^2 = \kappa^2\,\|P_1\boldsymbol{g}\|^2. \tag{A.13}$$

We sum up all the terms in (A.5) and obtain

$$\left\|(I+J+h^2J^\kappa)g\right\|_a^2 \le \|g\|_a^2 + \alpha h^2 \|P_1 g\|^2 \le (1+\alpha h^2)\|g\|_a^2 \tag{A.14}$$

in which

$$\alpha = \lambda_2^2 u^2\theta + (1-\lambda_2)^2 \frac{\lambda_2}{2-\lambda_2} u^2\theta - 2\kappa + h^2\kappa^2 = \frac{\lambda_2}{2-\lambda_2} u^2\theta - 2\kappa + h^2\kappa^2. \tag{A.15}$$

Further we can see

$$\left\|I+J+h^2J^\kappa\right\|_a = \sup_{g\in\mathbb{R}^N} \frac{\left\|(I+J+h^2J^\kappa)g\right\|_a}{\|g\|_a} \le \sqrt{1+\alpha h^2} \tag{A.16}$$

and

$$\left\|I+J+h^2J^\kappa\right\|_{a,\Omega} \le \sqrt{1+\alpha_\infty h^2}, \tag{A.17}$$

where, in general,

$$\alpha_\infty = \frac{\lambda_2}{2-\lambda_2} u_\infty^2\theta + 2\kappa_\infty + h^2\kappa_\infty^2, \tag{A.18}$$

with

$$u_\infty = \max_{(t,x)\in[0,T]\times\Omega} |u(t,x)|, \quad \kappa_\infty = \max_{(t,x)\in[0,T]\times\Omega} |\kappa(t,x)|. \tag{A.19}$$

For the special case $\kappa \ge 0$ and $h \le \sqrt{2/\kappa_\infty}$, we can use the more refined estimate based on

$$\alpha_\infty = \frac{\lambda_2}{2-\lambda_2} u_\infty^2 \theta \tag{A.20}$$

because $-2\kappa + h^2\kappa^2 \le 0$ under these assumptions. Finally it is noted that $\lambda_2 = \gamma_2$ (see Theorem 4.1).

References

[1] M. K. Banda, W.-A. Yong, and A. Klar. A stability notion for lattice Boltzmann equations. SIAM J. Sci. Comput, 27:2098–2111, 2006.

[2] P. Bhatnagar, E. Gross, and M. Krook. A model for collision processes in gases i: small amplitude processes in charged and neutral one-component system. Phys. Rev., 94:511–525, 1954.

[3] R. Blaak and P. M. A. Sloot. Lattice dependence of reaction-diffusion in lattice Boltzmann modeling. Comput. Phys. Commun., 129(1-3):256–266, 2000.

[4] R. Caflisch. The fluid dynamic limit of the nonlinear Boltzmann equation. Comm. Pure Appl. Math., 30:651–666, 1980.

[5] A. Caiazzo, M. Junk, and M. Rheinländer. Comparison of analysis techniques for the lattice Boltzmann method. Comput. Math. Appl., 58:883–897, 2009.

[6] S. Chen and G.D. Doolen. Lattice Boltzmann method for fluid flows. Annu. Rev. Fluid Mech., 30:329–364, 1998.

[7] S. Dellacherie. Construction and analysis of lattice Boltzmann methods applied to a 1d convection-diffusion equation. Acta. Appl. Math., 2013.

[8] I. Ginzburg. Equilibrium-type and link-type lattice Boltzmann models for generic advection and anisotropic-dispersion equation. Advances in Water Resources, 28:1171–1195, 2005.

[9] M. Junk, A. Klar, and L.-S. Luo. Asymptotic analysis of the lattice Boltzmann equation. J. Comput. Phys., 210:676–704, 2005.

[10] M. Junk and Z. Yang. Asymptotic analysis of lattice Boltzmann boundary conditions. J. Stat. Phys., 121:3–35, 2005.

[11] M. Junk and Z. Yang. Convergence of lattice Boltzmann methods for Stokes flows in periodic and bounded domains. Comput. Math. Appl., 55(7):1481–1491, 2008.

[12] M. Junk and Z. Yang. Convergence of lattice Boltzmann methods for Navier-Stokes flows in periodic and bounded domains. Numerische Mathematik, 112(1):65–87, 2009.

[13] M. Junk and W.-A. Yong. Rigorous Navier-Stokes limit of the lattice Boltzmann equation. Asymp. Anal., 35:165–185, 2003.

[14] M. Junk and W.-A. Yong. Weighted L^2 stability of the lattice Boltzmann equation. SIAM J. Numer. Anal., 47:1651–1665, 2009.

[15] A. D. Masi, R. Esposito, and J. L. Lebowitz. Incompressible Navier-Stokes and Euler limits of the Boltzmann equation. Comm. Pure Appl. Math., 42(8):1189–1214, 1989.

[16] S. P. Dawson, S. Chen, and G. D. Doolen. Lattice Boltzmann computations for reactiondiffusion equations. The Journal of Chemical Physics, 98(2):1514–1523, 1993.

[17] M. Rheinländer. Analysis of Lattice-Boltzmann Methods :Asymptotic and Numeric Investigation of a Singularly Perturbed System. Dissertation, 2007.

[18] B. Shi and Z. Guo. Lattice Boltzmann model for nonlinear convection-diffusion equations. Phys. Rev. E, 79:016701, 2009.

[19] M. Stiebler, J. Tölke, and M. Krafczyk. Advection-diffusion lattice Boltzmann scheme for hierarchical grids. Comput. Math. Appl., 55(7):1576–1584, 2008.

[20] G. Strang. Accurate partial difference methods ii. non-linear problems. Numeric Mathematik, 6:37–64, 1964.

[21] J. Wang, D. Wang, P. Lallemand, and L.-S. Luo. Lattice Boltzmann simulations of thermal convective flows in two dimensions. Comput. Math. Appl., 65(2):262–286, 2013.

[22] J.-P. Weiß. Numerical Analysis of Lattice Boltzmann Methods for the Heat Equation on a Bounded Interval. Dissertation, 2006.

[23] H. Yoshida and M. Nagaoka. Multiple-relaxation-time lattice Boltzmann model for the convection and anisotropic diffusion equation. J. Comput. Phys., 229(20):7774–7795, 2010.