

## Analysis and Invariant Properties of a Lattice Boltzmann Method

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**Abstract.** We investigate a two-relaxation-time (TRT) lattice Boltzmann algorithm with the asymptotic analysis technique. The results are used to analyze invariance properties of the method. In particular, we focus on time dependent Stokes and Navier-Stokes problems.

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### 1 Introduction

The investigations reported here are motivated by the seminal paper [6,8] on the two-relaxation-time (TRT) lattice Boltzmann algorithm. Compared to the full MRT collision operator [4,5,11,17], the TRT approach has the advantage of being much closer in spirit to a BGK operator which alleviates the implementation and improves the efficiency of the algorithm. On the other hand, it outperforms the BGK [2] method because the extra relaxation parameter which is not required for consistency can be used to improve the stability, to reduce certain error terms or to achieve specific invariances.

The latter case has been carefully studied in [6] where the TRT algorithm is used to approximate the stationary Stokes or Navier-Stokes equation and where certain invariances of the algorithm are explained in detail. To see more clearly, which aspects of the algorithm lead to a loss of these invariance in case of the instationary equations is one goal of the present work.

We approach this goal by deriving the equation for the leading order error of the TRT algorithm using the asymptotic analysis method [12,14,19]. One advantage of this approach is the very transparent explanation of the relation between the lattice Boltzmann output and the solution of the incompressible Stokes or Navier-Stokes equation

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which can even be used for a convergence proof [15, 16]. Secondly, the fact that the asymptotic analysis is based on a regular expansion with coefficients that are fully expanded (as opposed to the Chapman Enskog approach [1, 5, 7]) allows to easily derive necessary conditions for invariances of the underlying algorithm.

Compared to earlier works, we present a simplification of the asymptotic analysis which is also related to invariance properties. In fact, whenever the solution of a singularly perturbed equation satisfies an additional, dependent relation which becomes independent in the limit, the asymptotic analysis can be simplified. Since the lattice Boltzmann algorithm can be viewed as a discretization of a singularly perturbed finite velocity Boltzmann equation with mass and momentum balance as additional relation, this idea can be employed.

We conclude the introduction with a short outline of the article. In section 2 we introduce several examples of invariances which will be considered later in case of the lattice Boltzmann algorithm. Moreover, we address how asymptotic analysis can be used to derive necessary conditions for invariance and how invariance properties can help in the analysis of singularly perturbed problems. In section 3, we introduce a complete TRT lattice Boltzmann algorithm, carry out the consistency analysis and close with a summary of the post processing needed to extract the Stokes or Navier-Stokes fields from the lattice Boltzmann variables. In the final section 4, we use the equation of the leading order error to check the invariance properties of the TRT algorithm with a special focus on the case of instationary equations.

## 2 Invariant properties

This article deals with some specific aspects of the general problem how to approximate equations  $E(U)=0$  which are accompanied by relevant additional conditions  $A(U)=0$ . We begin with some examples for this general framework, discuss numerical approximations on a general level and conclude with some comments on the analysis of lattice Boltzmann methods, which can benefit from using the availability of additional conditions.

### 2.1 Examples

#### 2.1.1 The harmonic oscillator

A famous example for an equation with meaningful additional condition is the harmonic oscillator

$$\ddot{U} + U = 0, \quad U(0) = 1, \quad \dot{U}(0) = 0,$$

where the total energy is conserved, i.e.

$$(\dot{U})^2 + U^2 = 1.$$

In our notation, the functions  $E$  and  $A$  would be

$$E(U) = \begin{pmatrix} \ddot{U} + U \\ U(0) - 1 \\ \dot{U}(0) \end{pmatrix}, \quad A(U) = (\dot{U})^2 + U^2 - 1.$$

Note that both  $E$  and  $A$  are defined on a suitable space of functions which is typical for problems involving differential equations. The formal conversion of equation and additional condition into expressions  $E$  and  $A$  should be clear from this example and will not be repeated in the following.

### 2.1.2 A finite velocity Boltzmann equation

A conservation invariant which plays an important role in this article comes along with the finite velocity Boltzmann equation

$$\frac{\partial}{\partial t} f_i + \mathbf{c}_i \nabla_x f_i = J_i(\mathbf{f}), \quad f_i|_{t=0} = \bar{f}_i, \quad (2.1)$$

posed, for simplicity on a periodic domain  $\Omega$ . We assume that there are  $N$  discrete velocities  $\mathbf{c}_i$  and that the collision operator  $J$  satisfies the conditions

$$\sum_{i=1}^N J_i(\mathbf{f}) = 0, \quad \sum_{i=1}^N J_i(\mathbf{f}) \mathbf{c}_i = 0.$$

which are responsible for local and global mass and momentum conservation. Introducing mass and momentum density as well as momentum flux

$$\rho = \sum_i f_i, \quad \mathbf{M} = \sum_i \mathbf{c}_i f_i, \quad \mathbf{P} = \sum_i \mathbf{c}_i \otimes \mathbf{c}_i f_i,$$

and the space averages

$$\bar{\rho} = \int_{\Omega} \rho \, dx, \quad \bar{\mathbf{M}} = \int_{\Omega} \mathbf{M} \, dx,$$

the conservation relations (which make up  $A$ )

$$\begin{aligned} \partial_t \rho + \nabla \cdot \mathbf{M} &= 0, & \frac{d}{dt} \bar{\rho} &= 0, \\ \partial_t \mathbf{M} + \nabla \cdot \mathbf{P} &= 0, & \frac{d}{dt} \bar{\mathbf{M}} &= 0, \end{aligned}$$

follow from (2.1) by multiplication with 1 and  $\mathbf{c}_i$  with subsequent summation over  $i$  and integration over  $\mathbf{x}$ .

### 2.1.3 Stationary Stokes equation

Apart from conservation relations, additional equations can also arise from a parametric independence as in the example of [6], where the viscosity independence of permeability computed from a Stokes simulation is considered. Here, the equation  $E(U)=0$  consists of the Stokes equation

$$\frac{1}{\varrho} \nabla p = \nu \Delta \mathbf{u}, \quad \nabla \cdot \mathbf{u} = 0,$$

for the unknown pressure and velocity  $U=(p, \mathbf{u})$  posed, for example, on a channel geometry containing obstacles with no-slip conditions  $\mathbf{u}=0$  at the rigid boundaries and finite pressure drop from inlet to outlet. Introducing the field  $\mathbf{w}=\nu \mathbf{u}$ , one observes that the  $\nu$ -derivatives  $p'$  and  $\mathbf{w}'$  of  $p$  and  $\mathbf{w}$  satisfy

$$\frac{1}{\varrho} \nabla p' = \Delta \mathbf{w}', \quad \nabla \cdot \mathbf{w}' = 0,$$

with homogeneous conditions on  $\mathbf{w}'$  and  $p'$  so that  $p' = 0$  and  $\mathbf{w}' = 0$ . This independence of  $\nu$  can be seen as an additional equation which entails the  $\nu$ -independence of permeability which is a derived quantity of  $p$  and  $\nu \mathbf{u}$ .

### 2.1.4 Instationary Stokes equation

A third class of invariances arises from scaling properties of the underlying equation. Our first example concerns the time dependent Stokes equation

$$\partial_t \mathbf{u} + \frac{1}{\varrho} \nabla p = \nu \Delta \mathbf{u} + \mathbf{g}, \quad \nabla \cdot \mathbf{u} = 0, \tag{2.2}$$

with a source term  $\mathbf{g}$  and, for example, zero initial and boundary values for velocity. Here, the solution shows a certain independence of viscosity, provided the time variable is suitably rescaled. To be more specific, we introduce the domain  $Q = [0, T_\nu] \times \Omega$  and the source

$$\mathbf{g}(t, \mathbf{x}) = \boldsymbol{\eta}\left(\frac{t}{T_\nu}, \mathbf{x}\right),$$

where  $\boldsymbol{\eta}$  is defined on  $[0, 1] \times \Omega$ . From the solution  $\mathbf{u}, p$  of (2.2), the transformed fields

$$\mathbf{v}(\tau, \mathbf{x}) = \nu \mathbf{u}(T_\nu \tau, \mathbf{x}), \quad q(\tau, \mathbf{x}) = p(T_\nu \tau, \mathbf{x}),$$

are constructed. For  $T_\nu = C/\nu$ , they satisfy the  $\nu$ -independent equation

$$\frac{1}{C} \partial_\tau \mathbf{v} + \frac{1}{\varrho} \nabla q = \Delta \mathbf{v} + \boldsymbol{\eta}, \quad \nabla \cdot \mathbf{v} = 0,$$

again with zero initial and boundary data for  $\mathbf{v}$ . In particular, we have the invariance property

$$\frac{\partial}{\partial \nu} \mathbf{v} = 0, \quad \frac{\partial}{\partial \nu} q = 0.$$

### 2.1.5 Navier-Stokes equation

The second example of scaling invariance arises from the classical non-dimensionalization of the Navier-Stokes equation

$$\partial_t \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \frac{1}{\rho} \nabla p = \nu \Delta \mathbf{u} + \mathbf{g}, \quad \nabla \cdot \mathbf{u} = 0. \tag{2.3}$$

We assume that (2.3) is posed on the domain  $Q = [0, T] \times \Omega$  which is obtained by scaling  $Q^* = [0, 1] \times \Omega^*$  with the factors  $T, L > 0$ , i.e.,  $[0, T] = T \cdot [0, 1]$  and  $\Omega = L \cdot \Omega^*$ . Also the data of the problem is defined by suitably scaling functions on  $Q^*$ . In particular, initial and boundary values are given by

$$\mathbf{u}(0, \mathbf{x}) = \bar{u} \boldsymbol{\psi} \left( \frac{\mathbf{x}}{L} \right), \quad \mathbf{u}(t, \mathbf{x}) = \bar{u} \boldsymbol{\phi} \left( \frac{t}{T}, \frac{\mathbf{x}}{L} \right), \quad \mathbf{x} \in \partial \Omega, \tag{2.4}$$

and the source term is

$$\mathbf{g}(t, \mathbf{x}) = \bar{g} \boldsymbol{\eta} \left( \frac{t}{T}, \frac{\mathbf{x}}{L} \right),$$

where  $\bar{u}, \bar{g} > 0$  are additional scaling factors. For completeness, we add a pressure scaling factor  $\bar{p} > 0$  to the list of relevant parameters

$$\pi = (T, L, \bar{u}, \bar{p}, \bar{g}, \rho, \nu) \in (0, \infty)^7 = \Pi.$$

Clearly, the solution  $U = (p, \mathbf{u})$  of the complete problem depends on  $\pi$  apart from  $(t, \mathbf{x})$  so that  $E$  operates on functions with domain of definition

$$\{(t, \mathbf{x}, \pi) \mid \pi \in \Pi, t \in [0, \pi_1], \mathbf{x} \in \pi_2 \Omega^*\}.$$

Now, scaling invariance means that a suitably scaled version of the solution

$$\mathbf{v}(\tau, \mathbf{y}, \pi) = \bar{u}^{-1} \mathbf{u}(T\tau, L\mathbf{y}, \pi), \tag{2.5a}$$

$$q(\tau, \mathbf{y}, \pi) = \bar{p}^{-1} p(T\tau, L\mathbf{y}, \pi), \tag{2.5b}$$

is constant on certain subsets of the parameter space. For the Navier-Stokes equation in our example, the subsets  $\Pi_{Re, Fr}$  are three dimensional manifolds in  $\Pi$  which are controlled by two parameters, the Reynolds number  $Re$  and the Froude number  $Fr$  through the relations

$$\frac{T\bar{u}}{L} = 1, \quad \frac{\bar{u}}{T\bar{g}} = Fr, \quad \frac{\bar{p}}{\rho\bar{u}^2} = 1, \quad \frac{\bar{u}L}{\nu} = Re. \tag{2.6}$$

In fact, it is easy to show using chain rule that, for  $\pi \in \Pi_{Re, Fr}$ , the fields  $\mathbf{v}, q$  satisfy

$$\partial_\tau \mathbf{v} + (\mathbf{v} \cdot \nabla_{\mathbf{y}}) \mathbf{v} + \nabla_{\mathbf{y}} q = \frac{1}{Re} \Delta_{\mathbf{y}} \mathbf{v} + \frac{1}{Fr} \boldsymbol{\eta}, \quad \nabla_{\mathbf{y}} \cdot \mathbf{v} = 0, \tag{2.7}$$

on  $Q^*$  with initial value  $\boldsymbol{\psi}$  and boundary value  $\boldsymbol{\phi}$  which is clearly independent of  $\pi \in \Pi_{Re, Fr}$ . Hence, if we parametrize  $\Pi_{Re, Fr}$  with three coordinates, the corresponding

derivatives of  $v$  and  $q$  are zero. For example, we could choose  $T, L, \bar{p}$  as coordinates so that

$$\frac{\partial}{\partial L}v = \frac{\partial}{\partial T}v = \frac{\partial}{\partial \bar{p}}v = 0, \quad \frac{\partial}{\partial L}q = \frac{\partial}{\partial T}q = \frac{\partial}{\partial \bar{p}}q = 0. \quad (2.8)$$

Altogether, this case of scaling invariance is subsumed in our general framework with  $E$  consisting of (2.3), (2.4) and  $A$  given by (2.8).

## 2.2 Numerical Methods

Having seen several explicit examples of equations accompanied by some invariance property, we now take an abstract point of view and suppose that the mathematical model  $E(U) = 0$  determines the unknown  $U$  uniquely and is accompanied by some other meaningful relation  $A(U) = 0$  which is automatically satisfied by  $U$ . Preserving this invariance property in a discretization process is generally desirable but difficult because the full set of equations  $E(U) = 0, A(U) = 0$  is an overdetermined system. In the case of finite volume schemes, for example, the conservative property is ensured first, by restricting to schemes of a specific structure. The remaining flexibility (choice of the numerical flux function) is then used to construct approximations of the actual equation with various degrees of accuracy.

Also in the lattice Boltzmann method, the algorithm is designed based on conservation properties. Depending on the choice of the collision model, however, the scheme may contain more parameters than required to assure consistency with the equations of fluid dynamics. In this case, one can try to use these extra parameters, to ensure additional invariance properties.

A method to check whether a free parameter is able to control the invariance property is offered by asymptotic analysis. To be more specific, we assume that the numerical solution  $U_h$  is determined by the approximated equation  $E_h(U_h) = 0$  where  $h > 0$  is a small parameter that controls the accuracy of the solution. Expanding  $U_h$  as

$$U_h = U^{(0)} + hU^{(1)} + h^2U^{(2)} + \dots,$$

inserting it into  $E_h$  and exploiting Taylor arguments, equations for the expansion coefficients are derived. Then, consistency of the algorithm amounts to the condition  $E(U^{(0)}) = 0$  while the order  $p$  of the method depends on whether  $U^{(1)}, \dots, U^{(p-1)}$  are forced to zero by their respective equations [13].

To derive a necessary condition for the fulfillment of the invariance property, we assume  $A(U_h) = 0$ , or maybe  $A_h(U_h) = 0$  for a discretized version if necessary. In the simpler case that  $A(U_h)$  is a meaningful expression, expansion yields

$$0 = A(U_h) = A(U^{(0)}) + hA'(U^{(0)})U^{(1)} + h^2 \left( A'(U^{(0)})U^{(2)} + \frac{1}{2}A''(U^{(0)})[U^{(1)}, U^{(1)}] \right) + \dots \quad (2.9)$$

The expression can only vanish for all  $h > 0$  if the contributions in different orders vanish separately, i.e.

$$\begin{aligned} A(U^{(0)}) &= 0, & A'(U^{(0)})U^{(1)} &= 0, \\ A'(U^{(0)})U^{(2)} + \frac{1}{2}A''(U^{(0)})[U^{(1)}, U^{(1)}] &= 0, & \dots \end{aligned}$$

In general some of these necessary conditions for the fulfillment of the constraint  $A(U_h) = 0$  are automatically satisfied. For example, if the scheme is consistent, the leading order  $A(U^{(0)})$  vanishes as it is automatically satisfied by solutions of  $E(U^{(0)}) = 0$ . Similarly, the conditions up to  $h^{p-1}$  are satisfied, if the scheme is consistent of order  $p$  because

$$U^{(1)} = \dots = U^{(p-1)} = 0,$$

in this case. Hence the first essential condition appears in order  $p$ . To explain the general procedure, let us assume that the scheme is first order accurate. Then the leading order necessary condition is

$$A'(U^{(0)})U^{(1)} = 0, \tag{2.10}$$

which has to be checked with the knowledge about the equations determining  $U^{(0)}$  and  $U^{(1)}$ . If free parameters can be used to ensure (2.10), then there is the chance that the scheme satisfies the additional condition. To get more confidence, checking the next order is an option but for complete certainty, a direct proof of  $A(U_h) = 0$  using the discrete equation  $E_h(U_h) = 0$  is mandatory. However, if (2.10) cannot be satisfied for any choice of the parameters, then the necessary condition is violated which means that invariance of the numerical scheme cannot be achieved. In this case, no additional argument is required. Thus, the asymptotic analysis is an easy way to check the potential of the free parameters.

We note in passing that the construction of the necessary conditions from (2.9) requires a complete expansion in terms of  $h$  because otherwise the expressions in the various orders need not be equal to zero separately. In contrast to the Chapman-Enskog expansion, the asymptotic analysis employed in section 3.2 delivers such a complete expansion.

### 2.3 Singular Limits

In the previous section, we have seen the role of asymptotic analysis in checking whether a numerical method satisfies some additional condition. Now we consider the reverse situation, how the fulfillment of additional conditions by the numerical solution can simplify the asymptotic analysis.

This situation generally occurs in the analysis of singularly perturbed equations and is due to the fact that for such systems the limit equations change type which leads to a loss of information. The expansion of the additional condition can then give important extra information and speed up the analysis process. Before exploiting this

property in case of lattice Boltzmann algorithms, we want to explain the strategy with a very simple linear model problem

$$\left(\frac{1}{\epsilon}B_0 + B_1\right)x = \frac{1}{\epsilon}b_\epsilon, \tag{2.11}$$

where

$$B_0 = \begin{pmatrix} 12 & 16 \\ -6 & -8 \end{pmatrix}, \quad B_1 = \begin{pmatrix} -4 & -8 \\ 3 & 6 \end{pmatrix},$$

and

$$b_\epsilon = \begin{pmatrix} -4/(1+\epsilon) \\ 2 \cos(\epsilon) \end{pmatrix} = \begin{pmatrix} -4 \\ 2 \end{pmatrix} + \epsilon \begin{pmatrix} 4 \\ 0 \end{pmatrix} + \mathcal{O}(\epsilon^2).$$

Since

$$\det\left(\frac{B_0}{\epsilon} + B_1\right) = \frac{8}{\epsilon},$$

Eq. (2.11) is uniquely solvable for every  $\epsilon > 0$ . Multiplying the equation with  $\epsilon$ , inserting the regular expansion

$$x = x_0 + \epsilon x_1 + \epsilon^2 x_2 + \dots,$$

and going to the limit  $\epsilon \rightarrow 0$  leads to the systems

$$B_0 x_0 = \begin{pmatrix} -4 \\ 2 \end{pmatrix}, \quad B_0 x_1 + B_1 x_0 = \begin{pmatrix} 4 \\ 0 \end{pmatrix}, \quad \dots,$$

where the first equation reads more explicitly

$$\begin{pmatrix} 12 & 16 \\ -6 & -8 \end{pmatrix} x_0 = \begin{pmatrix} -4 \\ 2 \end{pmatrix}.$$

The obvious linear dependence of the rows of  $B_0$  represents a typical behavior of singular limits: the leading order expansion coefficient  $x_0$  is not determined uniquely by the leading order limit equation. It may even happen that the regular expansion fails completely if the right hand side is not in the range of the leading order operator. In this case of incompatible data (which we are not facing here), the solution to the original problem has a more complicated (singular)  $\epsilon$ -dependence which cannot be described with the smooth polynomial dependence of the regular expansion.

In our specific case, we find

$$x_0 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} + \alpha_0 \begin{pmatrix} 4 \\ -3 \end{pmatrix}, \tag{2.12}$$

where  $\alpha_0$  is still undetermined. The missing information is hidden in the next order relation

$$B_0 x_1 = \begin{pmatrix} 4 \\ 0 \end{pmatrix} - B_1 x_0 = \begin{pmatrix} 0 \\ 3 \end{pmatrix} + \alpha_0 \begin{pmatrix} -8 \\ 6 \end{pmatrix},$$



which is only solvable if the right hand side is in the range of  $B_0$ . This is exactly the case when

$$\begin{pmatrix} 0 \\ 3 \end{pmatrix} + \alpha_0 \begin{pmatrix} -8 \\ 6 \end{pmatrix} = \lambda \begin{pmatrix} -2 \\ 1 \end{pmatrix},$$

which leads to  $\alpha_0 = -3/2$  and  $\lambda = -6$ . This fixes  $x_0$  completely and  $x_1$  partly as solution of

$$B_0 x_1 = \lambda \begin{pmatrix} -2 \\ 1 \end{pmatrix} = \begin{pmatrix} 12 \\ -6 \end{pmatrix}.$$

More specifically, we find

$$x_0 = \begin{pmatrix} -2 \\ 3/2 \end{pmatrix}, \quad x_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \alpha_1 \begin{pmatrix} 4 \\ -3 \end{pmatrix}.$$

Continuing in this way, the higher order coefficients can be determined according to the same pattern:  $x_k$  is partly determined by equation  $k$  and fully by equation  $k + 1$ .

Since the derivation of higher order equations may be a very time consuming task for more complicated systems, we want to stress the importance of additional knowledge  $A(x) = 0$  about the solution of (2.11). A useful information in this case is obtained from the fact that  $\begin{pmatrix} 1 & 2 \end{pmatrix}$  is a left eigenvector of the system matrix

$$\begin{pmatrix} 1 & 2 \end{pmatrix} \left( \frac{1}{\epsilon} B_0 + B_1 \right) = 2 \begin{pmatrix} 1 & 2 \end{pmatrix},$$

so that

$$A(x) = \begin{pmatrix} 2 & 4 \end{pmatrix} x - \begin{pmatrix} 1 & 2 \end{pmatrix} \frac{1}{\epsilon} b_\epsilon = 0,$$

holds for all solutions of (2.11). Expanding this relation in the limit  $\epsilon \rightarrow 0$  gives rise to the leading order condition

$$\begin{pmatrix} 2 & 4 \end{pmatrix} x_0 - 4 = 0.$$

Combined with (2.12), this implies without going to the next equation

$$-2 - 4\alpha_0 - 4 = 0, \quad \text{resp.} \quad \alpha_0 = \frac{-3}{2}.$$

In other words, a relation which is automatically satisfied by the solution of a singularly perturbed problem can turn into an independent condition in the limit and thus alleviate the asymptotic analysis.

However, not all additional conditions have this property. For example

$$\tilde{A}(x) = \begin{pmatrix} 12 & 16 \end{pmatrix} x - \begin{pmatrix} 3 & 4 \end{pmatrix} b_\epsilon = 0,$$

gives rise to the leading order limit

$$\begin{pmatrix} 12 & 16 \end{pmatrix} x_0 + 4 = 0,$$

which is satisfied by (2.12) without additional requirements on  $\alpha_0$ .

We conclude that the analysis of a singularly perturbed problem  $E_\epsilon(U) = 0$  can profit from additional information  $A_\epsilon(U) = 0$  provided  $A_\epsilon(U)$  captures some aspects of the solution which is not automatically contained in the leading order limit equation.

This observation is exploited in the following analysis of the lattice Boltzmann method. To explain the precise relation to our preceding discussion, we note that the classical lattice Boltzmann algorithm can be seen as a particular discretization of a scaled version of the finite velocity Boltzmann equation (2.1)

$$\frac{\partial}{\partial t} f_i + \frac{1}{\epsilon} c_i \nabla_x f_i = \frac{1}{\epsilon^2} J_i(f). \tag{2.13}$$

Integrating (2.13) along characteristics over the time interval  $[t, t + \Delta t]$ , we obtain

$$f_i(t + \Delta t, \mathbf{x} + c_i \frac{\Delta t}{\epsilon}) = f_i(t, \mathbf{x}) + \frac{1}{\epsilon^2} \int_0^{\Delta t} J_i(f)(t + s, \mathbf{x} + c_i \frac{s}{\epsilon}) ds.$$

Coupling the space and time step size to the scaling parameter  $\epsilon$  according to  $\Delta t = \epsilon^2$  and  $\Delta x = \epsilon$ , and approximating the integral by the rectangle rule with the integrand evaluated at the left point of the interval, we arrive at

$$f_i(t + \Delta t, \mathbf{x} + c_i \Delta x) \approx f_i(t, \mathbf{x}) + J_i(f)(t, \mathbf{x}), \tag{2.14}$$

which leads to a simple algorithm when  $\mathbf{x}$  is restricted to a spatial lattice  $\Delta x \mathbb{X}$  which is invariant under  $\Delta x c_i$ -translations. If we use  $\hat{f}_i(k, j)$  to approximate the value  $f_i(k\Delta t, j\Delta x)$ , then we obtain the lattice Boltzmann evolution [9, 10] from (2.14)

$$\hat{f}_i(k + 1, j + c_i) = \hat{f}_i(k, j) + J_i(\hat{f})(k, j). \tag{2.15}$$

The point of this brief derivation is to demonstrate the explicit connection between the lattice Boltzmann algorithm (2.15) and the finite discrete-velocity model equation (2.13) which already indicates a fundamental difficulty in the analysis: since the lattice Boltzmann equation (2.15) can be viewed as a discretization of the singularly perturbed equation (2.13) with coupled parameters  $\Delta t = \Delta x^2 = \epsilon^2$ , it is clear that the limit of vanishing discretization length  $\Delta x$  is a singular limit.

To alleviate the analysis, we search for additional equations which are automatically satisfied by the solution  $\hat{f}$  of (2.15). Similar to the continuous case discussed in section 2.1, such relations are offered by the conservation equations

$$\sum_i \left( \hat{f}_i(k + 1, j + c_i) - \hat{f}_i(k, j) \right) = 0, \tag{2.16a}$$

$$\sum_i \left( \hat{f}_i(k + 1, j + c_i) - \hat{f}_i(k, j) \right) c_i = 0. \tag{2.16b}$$

In the next section, we present the analysis of (2.15) and (2.16) with the TRT collision operator  $J_j$ . Similar results can also be derived in the MRT case (the analysis has been

carried out, for example, in [12, 14]). However, the TRT model has the advantage that the structure of the equations is much simpler because the collision operator depends only on a single free parameter  $\lambda^-$ . Its relation to the parameter  $\lambda^+$  which controls the Navier-Stokes viscosity is decisive for the invariance property of the scheme.

### 3 Analysis of the TRT model

Here, we consider the Two-Relaxation-Time (TRT) lattice Boltzmann method introduced in [8]. A structural requirement for this approach is a point symmetric discrete velocity set

$$\mathbf{V} = \{c_i : i = 1, \dots, N\} \subset \{-1, 0, 1\}^d,$$

which means that with  $c_i \in \mathbf{V}$  also the opposite velocity  $c_{i^*} = -c_i$  is contained in  $\mathbf{V}$ . Based on this property, any function  $F : c_i \mapsto F_i$  of the discrete velocities can be decomposed into a symmetric (even) and an anti-symmetric (odd) component, i.e.,

$$F_i = F_i^+ + F_i^-,$$

with

$$F_i^+ = \frac{1}{2}(F_i + F_{i^*}), \quad F_i^- = \frac{1}{2}(F_i - F_{i^*}). \quad (3.1)$$

The collision operator  $J_i$  of the TRT model is a relaxation operator with two characteristic relaxation rates  $\lambda^+$  and  $\lambda^-$  both from the interval  $(-2, 0)$  which drives the odd and even parts of the particle distribution function  $\hat{f}_i$  towards suitable equilibrium values  $e_i^+$  and  $e_i^-$ . Introducing the difference between  $\hat{f}_i^\pm$  and  $e_i^\pm$  as non-equilibrium distributions

$$n_i^\pm = \hat{f}_i^\pm - e_i^\pm,$$

the collision operator has the general form

$$J_i = \lambda^+ n_i^+ + \lambda^- n_i^-. \quad (3.2)$$

For a complete specification of  $J_i$ , it remains to define the structure of the equilibrium values  $e_i$ . They depend on the particle distribution function  $f_i$  only through the velocity averages

$$\hat{\rho} = \sum_{i=1}^N \hat{f}_i, \quad \hat{\mathbf{M}} = \sum_{i=1}^N c_i \hat{f}_i, \quad (3.3)$$

which represent mass and momentum density at each lattice node. More specifically, we have

$$\begin{aligned} e_i^- &= 3w_i \hat{\mathbf{M}} \cdot c_i, \\ e_i^+ &= w_i \left( \hat{\rho} + g_s E_i(\hat{\mathbf{M}}, \hat{\mathbf{M}}, \hat{\rho}) \right), \end{aligned} \quad (3.4)$$

with

$$E_i(\mathbf{v}, \mathbf{u}, \bar{\rho}) = \frac{3}{2\bar{\rho}} \left( 3(\mathbf{u} \cdot c_i)(\mathbf{v} \cdot c_i) - (\mathbf{u} \cdot \mathbf{v}) \right). \quad (3.5)$$

Since the nonlinear term  $E$  is only required when approximating the Navier-Stokes equation, the switching variable  $g_s$  is introduced. Consistency to the Stokes equation will be achieved for  $g_s = 0$  and to the Navier-Stokes equation for  $g_s = 1$ . The weight function  $w_i$  is assumed to be symmetric, i.e.  $w_i = w_{i^*}$ , and should satisfy the following moment constraints

$$\sum_{i=1}^N w_i = 1, \quad \sum_{i=1}^N c_{i\alpha} c_{i\beta} w_i = \frac{1}{3} \delta_{\alpha\beta}, \tag{3.6}$$

$$\sum_{i=1}^N c_{i\alpha} c_{i\beta} c_{i\gamma} c_{i\delta} w_i = \frac{1}{9} (\delta_{\alpha\beta} \delta_{\gamma\delta} + \delta_{\alpha\delta} \delta_{\beta\gamma} + \delta_{\alpha\gamma} \delta_{\beta\delta}). \tag{3.7}$$

In the two dimensional case, possible weights are  $4/9$ ,  $1/9$  and  $1/36$  for the zero velocity, the velocities in coordinate directions and the diagonal directions respectively. The conditions ensure that

$$\sum_{i=1}^N e_i = \hat{\rho}, \quad \sum_{i=1}^N c_i e_i = \hat{M},$$

which leads to the conservation relations

$$\sum_{i=1}^N J_i = 0, \quad \sum_{i=1}^N c_i J_i = 0. \tag{3.8}$$

Having specified the collision operator, the remaining aspects of the lattice Boltzmann algorithm like the treatment of source terms as well as initial and boundary conditions are summarized below, followed by a detailed consistency analysis.

### 3.1 The algorithm

In this section, we introduce a lattice Boltzmann algorithm for the approximate solution of Stokes or Navier-Stokes problems on a domain  $Q = [0, T_e] \times \Omega$ . Our basic non-dimensional discretization parameter is  $h > 0$  from which we derive spatial and temporal step sizes according to

$$\Delta t = \hat{T} h^2, \quad \text{and} \quad \Delta x = \hat{L} h,$$

with positive parameters  $\hat{T}, \hat{L}$ . Approximations for the Stokes or Navier-Stokes fields are then computed at the discrete points  $(t_k, x_j) \in Q$  where  $t_k = k\Delta t$  is labeled by  $k \in \mathbb{N}_0$  and  $x_j = j\Delta x \in \Omega$  by suitable  $j \in \mathbb{Z}^d$ . We stress that the inbuilt relation  $\Delta t \sim \Delta x^2$  is crucial to capture the parabolic behavior of the Navier-Stokes equation with the explicit lattice Boltzmann algorithm.

For pairs  $j, j + c_i$  where the segment (the link) connecting the corresponding nodes is completely contained in the domain  $\Omega$ , the lattice Boltzmann rule for the update of the particle distribution function  $\hat{f}_i$  is a simple discrete advection

$$\hat{f}_i(k + 1, j + c_i) = \hat{f}_i^c(k, j), \tag{3.9}$$

where  $\hat{f}_i^c$  is the state after particle collision

$$\hat{f}_i^c(k, j) = \hat{f}_i(k, j) + \lambda^+ n_i^+(k, j) + \lambda^- n_i^-(k, j) + S_i(k, j). \quad (3.10)$$

The additional term  $S_i = S_i^+ + S_i^-$  is a prescribed external source term which may incorporate the macroscopic mass source (suppressed here) and the body force  $\varrho g$  of the hydrodynamic problem. A minimal requirement is

$$\sum_{i=1}^N S_i = 0, \quad \sum_{i=1}^N S_i c_i = \varrho \frac{\Delta t^2}{\Delta x} \mathbf{g}, \quad (3.11)$$

and the most simple way to ensure that is by setting

$$S_i^+ = 0, \quad S_i^- = \varrho \frac{\Delta t^2}{\Delta x} \mathbf{g}_i, \quad \mathbf{g}_i = 3w_i \mathbf{g} \cdot \mathbf{c}_i. \quad (3.12)$$

Another possibility, which turns out to be crucial for the enforcement of certain invariances, is described in [6,8]. It differs from (3.12) by the additional term

$$\Delta S_i = -w_i g_s \lambda^+ \left( E_i(\hat{\mathbf{M}}^s, \hat{\mathbf{M}}^s, \hat{\rho}) - E_i(\hat{\mathbf{M}}, \hat{\mathbf{M}}, \hat{\rho}) \right), \quad (3.13a)$$

$$\hat{\mathbf{M}}^s = \hat{\mathbf{M}} + \frac{\varrho \Delta t^2}{2\Delta x} \mathbf{g}, \quad (3.13b)$$

which satisfies

$$\sum_{i=1}^N \Delta S_i = 0, \quad \sum_{i=1}^N \Delta S_i c_i = 0,$$

so that (3.11) is still true when  $S_i$  is replaced by  $S_i + \Delta S_i$ . Effectively, the correction term (3.13) removes the contribution  $E_i(\hat{\mathbf{M}}, \hat{\mathbf{M}}, \hat{\rho})$  in (3.4) and replaces it by  $E_i(\hat{\mathbf{M}}^s, \hat{\mathbf{M}}^s, \hat{\rho})$ . In the following, we will therefore continue with the force term (3.12) but replace the equilibrium distribution (3.4) by

$$e_i^- = 3w_i \hat{\mathbf{M}} \cdot \mathbf{c}_i, \quad (3.14a)$$

$$e_i^+ = w_i \left( \hat{\rho} + g_s E_i(\hat{\mathbf{M}}^s, \hat{\mathbf{M}}^s, \hat{\rho}) \right). \quad (3.14b)$$

Since the modification does not influence the conservation relations (3.8), we have

$$\sum_{i=1}^N \hat{f}_i^c = \sum_{i=1}^N \hat{f}_i, \quad \sum_{i=1}^N c_i \hat{f}_i^c = \sum_{i=1}^N c_i \hat{f}_i + \varrho \frac{\Delta t^2}{\Delta x} \mathbf{g},$$

so that the solution of (3.9) and (3.10) satisfies the additional balance relations similar to (2.16)

$$\begin{aligned} \sum_i \left( \hat{f}_i(k+1, \mathbf{j} + \mathbf{c}_i) - \hat{f}_i(k, \mathbf{j}) \right) &= 0, \\ \sum_i \left( \hat{f}_i(k+1, \mathbf{j} + \mathbf{c}_i) - \hat{f}_i(k, \mathbf{j}) \right) c_i - \varrho \frac{\Delta t^2}{\Delta x} \mathbf{g} &= 0. \end{aligned} \quad (3.15)$$

at all interior nodes.

If the link between nodes  $j$  and  $j + c_i$  intersects the boundary at a point  $x_{ji}$ , the standard update rule is not feasible. To ensure velocity Dirichlet conditions, we adopt the bounce back algorithm

$$\hat{f}_i(k + 1, j) = \hat{f}_{i^*}^c(k, j) + 6w_i\varrho \frac{\Delta t}{\Delta x} \mathbf{u}_{bc}(t_k, \mathbf{x}_{ji}) \cdot \mathbf{c}_i, \tag{3.16}$$

To initialize  $\hat{f}_i$  one can use the equilibrium function  $e_i$  corresponding to the initial mass and momentum densities. In the case of non-constant initial fields, however, this approach generally leads to initial layers unless special modifications are incorporated [3, 18]. When the flow is driven by the source term or the boundary conditions, a very reasonable alternative is to smoothly switch on these conditions over time to avoid irregular behavior. For simplicity, we adopt this approach here, so that

$$\hat{f}_i(0, j) = w_i\varrho \tag{3.17}$$

with constant density  $\varrho > 0$  are initial values corresponding to constant pressure and zero flow velocity.

We remark in passing that, from the point of view of kinetic theory, the distribution  $w_i\varrho$  plays an important role because the incompressible Stokes or Navier-Stokes dynamics is obtained from the Boltzmann dynamics close to such constant states. In other words, if sources and boundary conditions are chosen in such a way that the density stays close to  $\varrho$  and the velocity stays close to zero, then the solution of the Boltzmann equation is essentially equivalent to a Stokes resp. Navier-Stokes solution. The smallness requirement is actually contained in the boundary condition (3.16) where  $\mathbf{u}_{bc}$  has the small prefactor

$$\frac{\Delta t}{\Delta x} \sim h,$$

and in the definition (3.12) of the source term where

$$\frac{\Delta t^2}{\Delta x} \sim h^3.$$

### 3.2 Consistency analysis

In this section, we show in which sense the lattice Boltzmann algorithm described above gives rise to approximate Stokes resp. Navier-Stokes solutions. In view of the fact that the algorithm is obtained by discretizing a singularly perturbed equation with the perturbation parameter coupled to space and time step (see the derivation in section 2.3), it is plausible that the consistency analysis has to be combined with an asymptotic analysis to capture the behavior in the singular limit. Moreover, as discussed at the end of the previous section, the relation between kinetic and hydrodynamic solutions is expected if the kinetic state is close to a spatially constant state. This motivates an expansion of the numerical solution  $\hat{f}_i$  around  $f_{i,0} = w_i\varrho$

$$\hat{f}_i(k, j) = \varrho w_i + hf_{i,1}(t_k, \mathbf{x}_j) + h^2 f_{i,2}(t_k, \mathbf{x}_j) + \dots, \tag{3.18}$$

where each coefficient  $f_{i,m}(t, x)$  is a smooth function of the independent variables  $t$  and  $x$ . For the derived moment averages (3.3) we find accordingly

$$\begin{aligned} \hat{\rho} &= \rho_0 + h\rho_1 + h^2\rho_2 + \dots, \\ \hat{\mathbf{M}} &= \mathbf{M}_0 + h\mathbf{M}_1 + h^2\mathbf{M}_2 + \dots, \\ \hat{\mathbf{M}}^g &= \mathbf{M}_0^g + h\mathbf{M}_1^g + h^2\mathbf{M}_2^g + \dots, \end{aligned}$$

with

$$\rho_m = \sum_i f_{i,m}, \quad \mathbf{M}_m = \sum_i \mathbf{c}_i f_{i,m}, \quad \mathbf{M}_m^g = \mathbf{M}_m + \delta_{3,m} \frac{\rho \hat{T}^2}{2L} \mathbf{g}.$$

Similarly, the equilibrium function is expanded

$$e_i = e_{i,0} + he_{i,1} + h^2e_{i,2} + \dots, \tag{3.19a}$$

with

$$e_{i,m} = e_{i,m}^+ + e_{i,m}^- \tag{3.19b}$$

$$e_{i,m}^- = 3w_i \mathbf{M}_m \cdot \mathbf{c}_i, \tag{3.19c}$$

$$e_{i,m}^+ = w_i(\rho_m + g_s E_{i,m}). \tag{3.19d}$$

Here, the contribution  $E_{i,m}$  is due to the nonlinear part  $E_i(\hat{\mathbf{M}}^g, \hat{\mathbf{M}}^g, \hat{\rho})$  which depends quadratically on  $\hat{\mathbf{M}}^g$  and inverse proportionally on  $\hat{\rho}$ , requiring an additional Taylor expansion. This leads to functions

$$E_i^{(k)}(\mathbf{w}, \mathbf{u}, \bar{\rho}) = \frac{1}{k!} \frac{\partial^k}{\partial \bar{\rho}^k} E_i(\mathbf{w}, \mathbf{u}, \bar{\rho}).$$

which are accompanied with the  $k$ -th power of the density variation

$$\hat{\rho} - \rho_0 = h\rho_1 + h^2\rho_2 + \dots,$$

so that  $k$ -fold products  $\rho_{j_1} \cdots \rho_{j_k}$  with  $j_i \geq 1$  appear in the expansion with order  $h^l$  where  $j_1 + \cdots + j_k = l$ . A total order  $h^m$  results when the two velocity arguments of  $E_i^{(k)}$  contain coefficients  $\mathbf{M}_r^g, \mathbf{M}_s^g$  with  $r + s = m - l$ . Altogether, this leads to the expression

$$E_{i,m} = \sum_{I_m} E_i^{(k)}(\mathbf{M}_s^g, \mathbf{M}_r^g, \rho_0) \rho_{j_1} \cdots \rho_{j_k},$$

where  $I_m$  is the index set of all combinations  $r, s, k \in \mathbb{N}_0$  and  $j_1, \dots, j_k \in \mathbb{N}$  with the property

$$r + s + j_1 + \cdots + j_k = m.$$

Fortunately, most of the terms disappear in the relevant orders of our investigation.

Finally, the non-equilibrium distributions are also split into the contributions at different orders

$$n_{i,m} = f_{i,m} - e_{i,m}, \quad n_{i,m}^+ = f_{i,m}^+ - e_{i,m}^+, \quad n_{i,m}^- = f_{i,m}^- - e_{i,m}^-. \tag{3.20}$$

which completes the expansion of the post collisional distribution  $\hat{f}_i^c$  in (3.10). It remains to expand the transport step (3.9). Here, insertion of the expansion leads to expressions of the form

$$f_{i,m}(t_{k+1}, \mathbf{x}_{j+c_i}) = f_{i,m}(t_k + \Delta t, \mathbf{x}_j + \Delta x \mathbf{c}_i),$$

which can be Taylor expanded at the node  $(t_k, \mathbf{x}_j)$  with respect to the parameter  $h$  which controls the step size  $\Delta t = \hat{T}h^2$  and  $\Delta x = \hat{L}h$ . Equating the resulting expressions at order  $m$ , we arrive at the general expression

$$\sum_{K_m} \frac{\hat{T}^a \hat{L}^b}{a!b!} \partial_t^a (\mathbf{c}_i \cdot \nabla)^b f_{i,c} - \lambda^+ n_{i,m}^+ - \lambda^- n_{i,m}^- - \delta_{m,3} \frac{\rho \hat{T}^2}{\hat{L}} \mathbf{g}_i = 0, \tag{3.21}$$

where  $K_m$  is the index set of all combinations  $a, b, c \in \mathbb{N}_0$  with  $2a + b + c = m$  and  $2a + b \geq 1$ . Similarly, expansion of the balance equations (3.15) leads to

$$\sum_{K_m} \sum_{i=1}^N \frac{\hat{T}^a \hat{L}^b}{a!b!} \partial_t^a (\mathbf{c}_i \cdot \nabla)^b f_{i,c} = 0, \tag{3.22}$$

$$\sum_{K_m} \sum_{i=1}^N \mathbf{c}_i \frac{\hat{T}^a \hat{L}^b}{a!b!} \partial_t^a (\mathbf{c}_i \cdot \nabla)^b f_{i,c} - \delta_{m,3} \frac{\rho \hat{T}^2}{\hat{L}} \mathbf{g} = 0. \tag{3.23}$$

After full expansion, we can now process the resulting equations order by order.

### 3.2.1 Leading order $m = 0$

Since  $f_{i,0} = w_i \rho$  leads to  $\rho_0 = \rho$  and  $\mathbf{M}_0 = 0$ , we have

$$e_{i,0}^- = 0, \quad e_{i,0}^+ = w_i \rho, \quad n_{i,0}^+ = n_{i,0}^- = 0. \tag{3.24}$$

### 3.2.2 First order $m = 1$

Since  $K_1$  contains only the index combination  $a = 0, b = 1, m = 0$  and gradients of  $f_{i,0}$  vanish, (3.21) gives

$$\lambda^+ n_{i,1}^+ + \lambda^- n_{i,1}^- = 0, \quad i = 1, \dots, N. \tag{3.25}$$

Computing odd and even parts of this equation leads to

$$n_{i,1}^+ = n_{i,1}^- = 0, \tag{3.26}$$

and hence

$$f_{i,1} = e_{i,1}, \quad e_{i,1}^+ = w_i \rho_1, \quad e_{i,1}^- = 3w_i \mathbf{M}_1 \cdot \mathbf{c}_i. \tag{3.27}$$

Here we have used

$$E_{i,1} = 2E_i(\mathbf{M}_0, \mathbf{M}_1, \rho) + E_i^{(1)}(\mathbf{M}_0, \mathbf{M}_0, \rho) \rho_1 = 0,$$

because  $\mathbf{M}_0 = 0$ . The characteristic feature of a singular limit, that the expansion coefficient of order  $m$  is not fully determined by equation  $m$ , is visible in relation (3.27)



because  $f_{i,1}$  is determined only up to its moments  $\rho_1$  and  $\mathbf{M}_1$ . As discussed in section 2.3, the additional balance equations (3.15) resp. the expanded forms (3.22) and (3.23) are useful to reduce this lack of information. For  $m = 2$ , they give relevant information on  $f_{i,1}$

$$\sum_{i=1}^N (\mathbf{c}_i \cdot \nabla) f_{i,1} = 0, \quad \sum_{i=1}^N \mathbf{c}_i (\mathbf{c}_i \cdot \nabla) f_{i,1} = 0, \quad (3.28)$$

and in combination with (3.27), this leads to

$$\nabla \cdot \mathbf{M}_1 = 0, \quad \nabla \rho_1 = 0. \quad (3.29)$$

### 3.2.3 Second order $m = 2$

Information on  $f_{i,2}$  is contained in (3.21) for  $m = 2$  and in (3.22) and (3.23) for  $m = 3$

$$\hat{L}(\mathbf{c}_i \cdot \nabla) f_{i,1} - \lambda^+ n_{i,2}^+ - \lambda^- n_{i,2}^- = 0, \quad (3.30)$$

$$\sum_{i=1}^N [(\hat{L} \mathbf{c}_i \cdot \nabla) f_{i,2} + \hat{T} \partial_t f_{i,1} + \hat{L}^2 \frac{1}{2} (\mathbf{c}_i \cdot \nabla)^2 f_{i,1}] = 0, \quad (3.31)$$

$$\sum_{i=1}^N \mathbf{c}_i [(\hat{L} \mathbf{c}_i \cdot \nabla) f_{i,2} + \hat{T} \partial_t f_{i,1} + \hat{L}^2 \frac{1}{2} (\mathbf{c}_i \cdot \nabla)^2 f_{i,1}] - \frac{\varrho \hat{T}^2}{\hat{L}} \mathbf{g} = 0. \quad (3.32)$$

Taking odd and even part of (3.30) and using (3.27), we find

$$n_{i,2}^+ = \hat{L} \frac{1}{\lambda^+} (\mathbf{c}_i \cdot \nabla) f_{i,1}^- = \hat{L} \frac{1}{\lambda^+} (\mathbf{c}_i \cdot \nabla) e_{i,1}^-, \quad (3.33a)$$

$$n_{i,2}^- = \hat{L} \frac{1}{\lambda^-} (\mathbf{c}_i \cdot \nabla) f_{i,1}^+ = 0. \quad (3.33b)$$

In the second equation of (3.33),  $\nabla \rho_1 = 0$  has been substituted. As a direct consequence,  $f_{i,2}$  has the form

$$f_{i,2} = e_{i,2} + n_{i,2}^+, \quad (3.34)$$

where  $e_{i,2}^+$  contains the term  $E_i(\mathbf{M}_1, \mathbf{M}_1, \varrho)$ . Insertion into Eq. (3.31) leads to

$$\hat{L} \nabla \cdot \mathbf{M}_2 + \hat{T} \partial_t \rho_1 = 0. \quad (3.35)$$

Noting that

$$\sum_{i=1}^N \mathbf{c}_i (\mathbf{c}_i \cdot \nabla) f_{i,2}^- = 0, \quad (3.36a)$$

$$\sum_{i=1}^N \mathbf{c}_i (\mathbf{c}_i \cdot \nabla) e_{i,2}^+ = \frac{1}{3} \nabla \rho_2 + \frac{\mathfrak{g}_s}{\varrho} (\mathbf{M}_1 \cdot \nabla) \mathbf{M}_1, \quad (3.36b)$$

$$\sum_{i=1}^N \mathbf{c}_i (\mathbf{c}_i \cdot \nabla)^2 e_{i,1}^- = \frac{1}{3} \Delta \mathbf{M}_1, \quad (3.36c)$$

Eq. (3.32) finally yields

$$\hat{T}\partial_t \mathbf{M}_1 + \frac{\hat{L}}{3}\nabla\rho_2 + \frac{\hat{L}g_s}{\varrho}(\mathbf{M}_1 \cdot \nabla)\mathbf{M}_1 = -\frac{1}{3}\left(\frac{1}{2} + \frac{1}{\lambda^+}\right)\hat{L}^2\Delta\mathbf{M}_1 + \frac{\varrho\hat{T}^2}{\hat{L}}\mathbf{g}, \quad (3.37)$$

which, up to some scalar factors, resembles the Navier-Stokes equation.

### 3.2.4 Higher orders $m = 3, m = 4$

Proceeding to the higher order terms, the computations get more lengthy but follow exactly the steps outlined for the lower order cases. Eventually, we obtain from (3.21)

$$n_{i,3}^+ = \frac{1}{\lambda^+} \left[ \hat{L}(\mathbf{c}_i \cdot \nabla)f_{i,2}^- + \hat{T}\partial_t f_{i,1}^+ \right], \quad (3.38a)$$

$$n_{i,3}^- = \frac{1}{\lambda^-} \left[ \hat{L}(\mathbf{c}_i \cdot \nabla)f_{i,2}^+ + \hat{T}\partial_t f_{i,1}^- + \frac{\hat{L}^2}{2}(\mathbf{c}_i \cdot \nabla)^2 f_{i,1}^- - \frac{\hat{T}^2}{\hat{L}}g_i \right], \quad (3.38b)$$

$$n_{i,4}^+ = \frac{1}{\lambda^+} \left[ \hat{L}(\mathbf{c}_i \cdot \nabla)f_{i,3}^- + (\hat{T}\partial_t + \frac{\hat{L}^2}{2}(\mathbf{c}_i \cdot \nabla)^2)f_{i,2}^+ \right] \quad (3.38c)$$

$$+ (\hat{T}\hat{L}\partial_t(\mathbf{c}_i \cdot \nabla) + \frac{\hat{L}^3}{6}(\mathbf{c}_i \cdot \nabla)^3)f_{i,1}^- \Big], \quad (3.38d)$$

$$n_{i,4}^- = \frac{1}{\lambda^-} \left[ \hat{L}(\mathbf{c}_i \cdot \nabla)f_{i,3}^+ + (\hat{T}\partial_t + \frac{\hat{L}^2}{2}(\mathbf{c}_i \cdot \nabla)^2)f_{i,2}^- \right]. \quad (3.38e)$$

Moreover, (3.22) and (3.23) show that the moments  $\mathbf{M}_2$  and  $\rho_3$  are governed by the homogeneous Oseen-type equation,

$$\begin{aligned} &\hat{T}\partial_t \mathbf{M}_2 + \frac{\hat{L}}{3}\nabla\rho_3 + \frac{\hat{L}g_s}{\varrho}[(\mathbf{M}_1 \cdot \nabla)\mathbf{M}_2 + (\mathbf{M}_2 \cdot \nabla)\mathbf{M}_1] \\ &= -\frac{1}{3}\left(\frac{1}{2} + \frac{1}{\lambda^+}\right)\hat{L}^2\Delta\mathbf{M}_2. \end{aligned} \quad (3.39)$$

and, similarly, that  $\mathbf{M}_3$  and  $\rho_4$  solve an Oseen-type problem which is generally non-homogeneous

$$\hat{L}\nabla \cdot \mathbf{M}_3 + \hat{T}\partial_t \rho_2 + \frac{\varrho\hat{T}^2}{2}\nabla \cdot \mathbf{g} = 0, \quad (3.40a)$$

$$\begin{aligned} &\hat{T}\partial_t \mathbf{M}_3 + \frac{\hat{L}}{3}\nabla\rho_4 + \frac{\hat{L}g_s}{\varrho}[(\mathbf{M}_1 \cdot \nabla)\mathbf{M}_3^g + (\mathbf{M}_3^g \cdot \nabla)\mathbf{M}_1] \\ &= -\frac{1}{3}\left(\frac{1}{2} + \frac{1}{\lambda^+}\right)\hat{L}^2\Delta\mathbf{M}_3 + R. \end{aligned} \quad (3.40b)$$

The source term  $R$  depends on the Navier-Stokes solutions and the body force  $\varrho\mathbf{g}$ . Following [6], we introduce

$$\Lambda_e = -\left(\frac{1}{\lambda^+} + \frac{1}{2}\right), \quad \Lambda_o = -\left(\frac{1}{\lambda^-} + \frac{1}{2}\right), \quad \Lambda_{eo} = \Lambda_e\Lambda_o. \quad (3.41)$$

Then  $R = R_0 + R_t$  can be written as

$$\begin{aligned}
 R_t &= \hat{T}\hat{L}(\Lambda_e + \Lambda_o)\partial_t\left(\frac{1}{3}\nabla\rho_2 + \frac{\mathcal{G}^s}{\varrho}(\mathbf{M}_1 \cdot \nabla)\mathbf{M}_1\right) + \hat{T}^2\Lambda_o\partial_t^2\mathbf{M}_1 - 2\hat{T}\hat{L}\frac{1}{3}\Lambda_e\partial_t\nabla\rho_2 \\
 &\quad + \frac{\varrho\hat{T}^3}{\hat{L}}\left(\Lambda_o + \frac{1}{2}\right)\partial_t\mathbf{g} - \hat{T}\hat{L}^2\left(\Lambda_e^2 + 2\Lambda_{eo} - \frac{1}{4}\right)\partial_t\left(\frac{1}{3}\Delta\mathbf{M}_1\right), \\
 R_0 &= -\hat{L}^3\left(\Lambda_{eo} - \frac{1}{12}\right)\left(\frac{1}{3}\nabla\Delta\rho_2 + \Delta(\mathbf{M}_1 \cdot \nabla)\mathbf{M}_1 + \frac{\mathcal{G}^s}{\varrho}D_3(\mathbf{M}_1, \mathbf{M}_1)\right) + \hat{L}^4\Lambda_e(\Lambda_{eo} \\
 &\quad - \frac{1}{6})\left(\frac{1}{3}\Delta^2\mathbf{M}_1 + D_4(\mathbf{M}_1)\right) + \varrho\hat{L}\hat{T}^2\frac{\Lambda_e}{3}\left(\Lambda_o + \frac{1}{2}\right)\Delta\mathbf{g} + \frac{2}{3}\varrho\hat{T}^2\hat{L}\Lambda_{eo}\nabla(\nabla \cdot \mathbf{g}),
 \end{aligned}$$

where  $R_0$  contains pure space derivatives and  $R_t$  collects the terms with time derivatives. Using equation (3.37), we can simplify these formulas to

$$R_t = -\Lambda_e\hat{T}^2\partial_t^2\mathbf{M}_1 + \frac{2}{3}\hat{T}\hat{L}^2\Lambda_{eo}\partial_t(\Delta\mathbf{M}_1) + \frac{\varrho\hat{T}^3}{\hat{L}}\left(\Lambda_e + 2\Lambda_o + \frac{1}{2}\right)\partial_t\mathbf{g} - 2\hat{T}\hat{L}\frac{1}{3}\Lambda_e\partial_t\nabla\rho_2, \tag{3.42}$$

$$\begin{aligned}
 R_0 &= \frac{\varrho\hat{T}^2\hat{L}}{12}(1 + 2\Lambda_e - 8\Lambda_{eo})\Delta\mathbf{g} + \frac{2}{3}\varrho\hat{T}^2\hat{L}\Lambda_{eo}\nabla(\nabla \cdot \mathbf{g}) - \hat{L}^4\frac{\Lambda_e}{36}\Delta^2\mathbf{M}_1 \\
 &\quad + \hat{L}^4\Lambda_e\left(\Lambda_{eo} - \frac{1}{6}\right)D_4(\mathbf{M}_1) - \hat{L}^3\left(\Lambda_{eo} - \frac{1}{12}\right)\frac{\mathcal{G}^s}{\varrho}D_3(\mathbf{M}_1, \mathbf{M}_1). \tag{3.43}
 \end{aligned}$$

For the subsequent investigations it will not be necessary to specify the precise structure of the differential expressions  $D_4(\mathbf{M}_1)$  and  $D_3(\mathbf{M}_1, \mathbf{M}_1)$ . It suffices to say that  $D_4$  is a linear differential operator of order 4 with respect to the spatial variables and that  $D_3(\mathbf{M}_1, \mathbf{M}_1)$  depends quadratically on  $\mathbf{M}_1$ , involving three space derivatives. Based on this information, we can tell how the expressions behave under scaling which is relevant for the investigation of scaling related invariances.

### 3.2.5 Initial conditions

Expansion of our simple initial condition (3.17) yields

$$f_{i,0}(0, \mathbf{x}) = \varrho w_i, \quad 0 = f_{i,1}(0, \mathbf{x}) = f_{i,2}(0, \mathbf{x}) = \dots$$

For the moments, this has the consequence  $\rho_0(0, \mathbf{x}) = \varrho$  and  $\rho_m(0, \mathbf{x}) = 0$  for all other  $m$ , as well as  $\mathbf{M}_m(0, \mathbf{x}) = 0$  for all  $m$ .

It should be noted, however, that these conditions are compatible with the expansion obtained from the update rule only under certain conditions. For example,  $\rho_2 = 0$  and  $\mathbf{M}_1 = 0$  at  $t = 0$  imply in connection with (3.37)

$$\partial_t\mathbf{M}_1(0, \mathbf{x}) = \varrho\frac{\hat{T}}{\hat{L}}\mathbf{g}(0, \mathbf{x}).$$

Applying the divergence and taking (3.29) into account, we arrive at the condition

$$\nabla \cdot \mathbf{g}(0, \mathbf{x}) = 0. \tag{3.44}$$

A violation of this condition enforces a discontinuity of some expansion coefficients at  $t = 0$  which is a contradiction to the smoothness assumption and implies that the

behavior of the algorithm cannot be described properly with smooth functions alone. From this observation we can tell, that a non-smooth behavior (initial layer) occurs, if (3.44) is not met. The behavior can be avoided by suitably changing the initial condition or by requiring (3.44). We stick to the latter option to keep the analysis (and the LB scheme) simple. In fact, we even adopt the somewhat stronger condition  $g(0, \mathbf{x}) = 0$  to simplify the considerations later on.

### 3.2.6 Boundary conditions

It remains to derive the boundary values of the relevant moments which we obtain by inserting the expansion (3.18) into (3.16) and later using the specific form of the coefficients which we have already computed.

Expanding around the point  $(t_k, \mathbf{x}_{ji})$  generally involves a shift

$$\mathbf{x}_{ji} = \mathbf{x}_j + q_{ji}\Delta x \mathbf{c}_i \in \partial\Omega,$$

from the lattice node  $\mathbf{x}_j$  with space increment  $q_{ji}\Delta x$  along  $\mathbf{c}_i$  where  $q_{ji} \in [0, 1)$ . Therefore the expansion of  $f_{i,m}(t_{k+1}, \mathbf{x}_j)$  involves both space and time derivatives as in the case of the update rule. In addition, a spatial Taylor expansion of the post collisional distribution appears. After collecting terms of equal order, we obtain at  $(t_k, \mathbf{x}_{ji})$

$$\begin{aligned} \sum_{2a+b+c=m} \frac{\hat{T}^a \hat{L}^b q_{ji}^b}{a!b!} \partial_i^a (\mathbf{c}_i \cdot \nabla)^b f_{i,c} - \sum_{b+c=m} \frac{\hat{L}^b q_{ji}^b}{b!} (\mathbf{c}_i \cdot \nabla)^b (f_{i^*,c} \\ + \lambda^+ n_{i^*,c}^+ + \lambda^- n_{i^*,c}^- + \frac{\hat{T}^2}{\hat{L}} g_{i^*} \delta_{3,c}) = \beta_i \delta_{1,m}, \end{aligned} \tag{3.45}$$

where  $\beta_i = 6\hat{T}/\hat{L} w_i \varrho \mathbf{u}_{bc} \cdot \mathbf{c}_i$ . For the relevant orders, this implies

$$f_{i,1} = f_{i^*,1} + 6w_i \varrho \frac{\hat{T}}{\hat{L}} \mathbf{u}_{bc} \cdot \mathbf{c}_i, \tag{3.46a}$$

$$f_{i,2} = f_{i^*,2} + \hat{L}(1 - 2q_{ji})(\mathbf{c}_i \cdot \nabla) e_{i,1}^-, \tag{3.46b}$$

$$\begin{aligned} f_{i,3} = f_{i^*,3} + \lambda^+ n_{i^*,3}^+ + \lambda^- n_{i^*,3}^- + \frac{\hat{T}^2}{\hat{L}} g_{i^*} - \hat{T} \partial_t f_{i,1} \\ - 2q_{ji} \hat{L} (\mathbf{c}_i \cdot \nabla) e_{i,2}^- + q_{ji} (1 - q_{ji}) \hat{L}^2 (\mathbf{c}_i \cdot \nabla)^2 e_{i,1}^-. \end{aligned} \tag{3.46c}$$

Substituting the known form of  $f_{i,c}$  in detail, we find in leading order

$$\mathbf{M}_1 \cdot \mathbf{c}_i = \varrho \frac{\hat{T}}{\hat{L}} \mathbf{u}_{bc} \cdot \mathbf{c}_i, \tag{3.47}$$

which assigns, up to a factor, the boundary value  $\mathbf{u}_{bc}$  to the first order moment  $\mathbf{M}_1$ . However, the next relation

$$\mathbf{M}_2 \cdot \mathbf{c}_i = \frac{\hat{L}}{2} (1 - 2q_{ji})(\mathbf{c}_i \cdot \nabla)(\mathbf{M}_1 \cdot \mathbf{c}_i), \tag{3.48}$$

can, in general, not be satisfied for any choice of  $M_2$  because the left hand side is linear in  $c_i$  while the right hand side is quadratic. Only if  $q_{ji} = 1/2$ , which refers to certain grid adapted geometries, this problem does not appear. In the remaining cases, the contradiction implies that the smooth expansion (3.18) is unable to satisfy the relations defining the lattice Boltzmann algorithm, so that, inevitably, irregular terms of at least second order are present in the numerical solution. For a more detailed discussion of this phenomenon, we refer to [14].

In the following, we assume  $q_{ji} = 1/2$ , so that (3.48) enforces homogeneous boundary conditions for  $M_2$ . Alternatively, we could have picked a more accurate boundary condition than the bounce back rule but we refrained from doing so to keep the analysis more transparent. Combined with (3.35), the condition  $M_2 = 0$  on  $\partial\Omega$  helps to determine  $\rho_1$  fully. Since  $\rho_1$  is constant in space according to (3.29), integration of (3.35) over the domain  $\Omega$  yields

$$\begin{aligned} 0 &= \hat{T}|\Omega|\partial_t\rho_1 + \hat{L} \int_{\Omega} \nabla \cdot M_2 dx \\ &= \hat{T}|\Omega|\partial_t\rho_1 + \hat{L} \int_{\partial\Omega} M_2 \cdot n dx = \hat{T}|\Omega|\partial_t\rho_1. \end{aligned}$$

Combined with the initial value  $\rho_1(0, x) = 0$ , this implies  $\rho_1 = 0$  in space and time. Eq. (3.35) then turns into the incompressibility condition  $\nabla \cdot M_2 = 0$  for  $M_2$  and since (3.39) is also homogeneous, the zero initial and boundary conditions imply  $M_2 = 0$ , and  $\nabla\rho_3 = 0$ . Summarizing these observations, we conclude that the bounce back rule with  $q_{ji} = 1/2$  or any other second order accurate boundary condition implies

$$\rho_1 = 0, \quad M_2 = 0, \quad \nabla\rho_3 = 0. \quad (3.49)$$

Proceeding to the next equation

$$\begin{aligned} M_3 \cdot c_i &= \Lambda_o \frac{\hat{L}}{3} (c_i \cdot \nabla) [\rho_2 + g_s E_i(M_1, M_1, \rho)] + \frac{\hat{L}}{2} (1 - 2q_{ji}) (c_i \cdot \nabla) (M_2 \cdot c_i) \\ &+ \hat{T} (\Lambda_o - \frac{1}{2}) \partial_t (M_1 \cdot c_i) - \frac{\hat{L}^2}{2} [2\Lambda_{eo} - q_{ji}(1 - q_{ji})] (c_i \cdot \nabla)^2 M_1 \cdot c_i \\ &- \frac{\varrho \hat{T}^2}{\hat{L}} (\Lambda_o + \frac{1}{2}) g \cdot c_i, \end{aligned} \quad (3.50)$$

we see that even in the case  $q_{ji} = 1/2$ , the required equality of a linear and a cubic expression in  $c_i$  is impossible to satisfy in general. A similar effect is also observed in all other boundary conditions which are only second order accurate. Hence, the regular expansion breaks down in third order. For checking invariances of the numerical solution, however, the equation is still useful as demonstrated below.

### 3.2.7 Extraction of hydrodynamics

From the complete analysis of the TRT lattice Boltzmann algorithm, we can now see how the hydrodynamic solution can be extracted. In view of section 3.2.1 and (3.49),

the expansion of the velocity averages has the form

$$\hat{\rho} = \rho + h^2 \rho_2 + \mathcal{O}(h^3), \quad \hat{\mathbf{M}} = h\mathbf{M}_1 + \mathcal{O}(h^3),$$

where  $\mathbf{M}_1, \rho_2$  satisfy Eq. (3.37) together with the incompressibility condition (3.29). Applying a proper scaling to  $\mathbf{M}_1, \rho_2$ , we can thus recover the Stokes or Navier-Stokes fields. More precisely, we set

$$\hat{\mathbf{u}} = \frac{1}{\rho} \frac{\Delta x}{\Delta t} \hat{\mathbf{M}}, \quad \hat{p} = \frac{\Delta x^2}{3\Delta t^2} (\hat{\rho} - \rho). \tag{3.51}$$

Then

$$\hat{p} = p + \mathcal{O}(h), \quad \hat{\mathbf{u}} = \mathbf{u} + \mathcal{O}(h^2),$$

where the leading order contributions  $p, \mathbf{u}$  satisfy the equations

$$\nabla \cdot \mathbf{u} = 0, \quad \partial_t \mathbf{u} + \frac{1}{\rho} \nabla p + g_s(\mathbf{u} \cdot \nabla) \mathbf{u} = \nu \Delta \mathbf{u} + \mathbf{g}, \tag{3.52}$$

with initial value  $\mathbf{u}(0, \mathbf{x}) = 0$ , boundary condition  $\mathbf{u}(t, \mathbf{x}) = \mathbf{u}_{bc}(t, \mathbf{x})$  and

$$\nu = -\frac{1}{3} \left( \frac{1}{2} + \frac{1}{\lambda^+} \right) \frac{\Delta x^2}{\Delta t} = \frac{\Lambda_\epsilon \hat{L}^2}{3 \hat{T}}. \tag{3.53}$$

Following [6,8], another way to define the hydrodynamic velocity field is

$$\hat{\mathbf{u}} = \frac{1}{\rho} \frac{\Delta x}{\Delta t} \left( \hat{\mathbf{M}} + \frac{\rho}{2} \frac{\Delta t^2}{\Delta x} \mathbf{g} \right), \quad \hat{p} = \frac{\Delta x^2}{3\Delta t^2} (\hat{\rho} - \rho). \tag{3.54}$$

Since  $\Delta t^2 / \Delta x \sim h^3$ , the modification has no consequence on the leading order contribution  $\mathbf{u}$  which still solves (3.52). It will turn out, however, that it is crucial to ensure certain invariance properties.

### 4 Invariance properties of the LB solution

In the following, we pick up some examples of parametric independence and scaling invariance discussed in section 2.1 and check whether the invariance may be preserved with the TRT lattice Boltzmann algorithm. From our observations in section 2.2, we know that an invariance of  $\hat{p}, \hat{\mathbf{u}}$  has implications on all expansion coefficients so that the hypothesis of invariance may be falsified by studying one particular order of expansion.

Using (3.54), we obtain

$$\hat{\mathbf{u}} = \mathbf{u} + h^2 \mathbf{u}_2 + \dots, \quad \hat{p} = p + h p_1 + h^2 p_2 + \dots,$$

with

$$\mathbf{u}_2 = \frac{\hat{L}}{\varrho \hat{T}} \left( \mathbf{M}_3 + \frac{\varrho \hat{T}^2}{2 \hat{L}} \mathbf{g} \right) = \frac{\hat{L}}{\varrho \hat{T}} \mathbf{M}_3^g, \quad p_1 = \frac{\hat{L}^2}{3 \hat{T}^2} \rho_3, \quad p_2 = \frac{\hat{L}^2}{3 \hat{T}^2} \rho_4.$$

The equation satisfied by  $\mathbf{u}_2$  and  $p_2$  follows from (3.40)

$$\nabla \cdot \mathbf{u}_2 + \frac{3 \hat{T}^2}{\varrho \hat{L}^2} \partial_t p = 0, \tag{4.1a}$$

$$\partial_t \mathbf{u}_2 + \frac{1}{\varrho} \nabla p_2 + g_s [(\mathbf{u} \cdot \nabla) \mathbf{u}_2 + (\mathbf{u}_2 \cdot \nabla) \mathbf{u}] = \nu \Delta \mathbf{u}_2 + \bar{R}. \tag{4.1b}$$

With our assumption  $\mathbf{g}(0, \mathbf{x}) = 0$ , and the conditions  $\mathbf{M}_3 = 0$ ,  $\rho_4 = 0$ , we see that both  $\mathbf{u}_2$  and  $p_2$  have zero initial values. Due to the inclusion of the acceleration term in  $\mathbf{u}_2$ , the source term  $R$  in Eq. (3.40) is modified to

$$\bar{R} = \frac{\hat{L}}{\varrho \hat{T}^2} R + \frac{\hat{T}}{2} \left[ \partial_t \mathbf{g} - \nu \Delta \mathbf{g} \right] = \bar{R}_t + \bar{R}_0. \tag{4.2}$$

Collecting again terms with time derivatives in  $\bar{R}_t$  and pure space derivatives in  $\bar{R}_0$ , we have

$$\bar{R}_t = -\Lambda_e \hat{T} \partial_t^2 \mathbf{u} + \frac{2}{3} \hat{L}^2 \Lambda_{eo} \partial_t (\Delta \mathbf{u}) + \hat{T} (\Lambda_e + 2\Lambda_o + 1) \partial_t \mathbf{g} - \frac{6\nu \hat{T}^2}{\varrho \hat{L}^2} \partial_t \nabla p, \tag{4.3}$$

$$\begin{aligned} \bar{R}_0 = & \frac{\hat{L}^2}{12} (1 - 8\Lambda_{eo}) \Delta \mathbf{g} + \frac{2}{3} \hat{L}^2 \Lambda_{eo} \nabla (\nabla \cdot \mathbf{g}) - \hat{L}^2 \frac{\nu}{12} \Delta^2 \mathbf{u} \\ & + \hat{L}^2 \frac{\nu}{2} (6\Lambda_{eo} - 1) D_4(\mathbf{u}) - g_s \hat{L}^2 (\Lambda_{eo} - \frac{1}{12}) D_3(\mathbf{u}, \mathbf{u}). \end{aligned} \tag{4.4}$$

Finally, the boundary condition for  $\mathbf{u}_2$  is, in the case  $q_{ji} = 1/2$ ,

$$\begin{aligned} \mathbf{u}_2 \cdot \mathbf{c}_i = & \Lambda_o \frac{\hat{L}}{3} (\mathbf{c}_i \cdot \nabla) \left[ \frac{3 \hat{T}}{\varrho \hat{L}} p + \frac{\hat{T}}{\hat{L}} g_s E_i(\mathbf{u}, \mathbf{u}, 1) \right] + \hat{T} (\Lambda_o - \frac{1}{2}) \partial_t (\mathbf{u} \cdot \mathbf{c}_i) \\ & - \hat{L}^2 \left( \Lambda_{eo} - \frac{1}{8} \right) (\mathbf{c}_i \cdot \nabla)^2 \mathbf{u} \cdot \mathbf{c}_i - \hat{T} \Lambda_o \mathbf{g} \cdot \mathbf{c}_i. \end{aligned} \tag{4.5}$$

In the following, we consider several special cases of the  $(\mathbf{u}_2, p_2)$ -equation. We begin with Stokes problems followed by a check of scaling invariance in the Navier-Stokes case.

### 4.1 Stationary Stokes equation

By setting  $g_s = 0$  in the Navier-Stokes algorithm, assuming time independent data and iterating to stationary, section 3.2.7 shows that properly scaled mass and momentum densities approximately satisfy the Stokes equation

$$\nabla \cdot \mathbf{u} = 0, \quad \frac{1}{\varrho} \nabla p = \nu \Delta \mathbf{u} + \mathbf{g}. \tag{4.6}$$

As discussed in section 2.1, solutions of (4.6) satisfy the additional property

$$\frac{\partial}{\partial \nu} p = 0, \quad \frac{\partial}{\partial \nu} (\nu \mathbf{u}) = 0,$$

provided  $\mathbf{g}$  is  $\nu$ -independent and  $\mathbf{u}_{bc} = 0$ . The corresponding invariance for a numerical solution  $\hat{p}, \hat{\mathbf{u}}$  would be

$$\frac{\partial}{\partial \nu} \hat{p} = 0, \quad \frac{\partial}{\partial \nu} (\nu \hat{\mathbf{u}}) = 0, \tag{4.7}$$

which is easily validated in case of standard finite difference or finite element approximations. For the TRT lattice Boltzmann scheme, however, the invariance is *not* automatically obtained but requires a particular definition of the relaxation parameter  $\lambda^-$  in relation to  $\lambda^+$ .

To see this, we first note that (4.7) implies

$$\frac{\partial}{\partial \nu} p_2 = 0, \quad \frac{\partial}{\partial \nu} (\nu \mathbf{u}_2) = 0,$$

upon insertion of the expansion. Introducing the field  $\mathbf{w}_2 = \nu \mathbf{u}_2$ , the equations for  $\mathbf{u}_2$  and  $p_2$  imply in the stationary case

$$\nabla \cdot \mathbf{w}_2 = 0, \quad \frac{1}{\varrho} \nabla p_2 = \Delta \mathbf{w}_2 + \bar{R}_0, \tag{4.8}$$

$$\begin{aligned} \bar{R}_0 = & \frac{\hat{L}^2}{12} (1 - 8\Lambda_{eo}) \Delta \mathbf{g} + \frac{2}{3} \hat{L}^2 \Lambda_{eo} \nabla (\nabla \cdot \mathbf{g}) \\ & - \hat{L}^2 \frac{1}{12} \Delta^2 (\nu \mathbf{u}) + \hat{L}^2 \frac{1}{2} (6\Lambda_{eo} - 1) D_4 (\nu \mathbf{u}). \end{aligned} \tag{4.9}$$

Since  $\mathbf{g}$  and  $\nu \mathbf{u}$  are independent of viscosity, we conclude

$$\frac{\partial}{\partial \nu} \bar{R}_0 = \frac{1}{3} \hat{L}^2 \Lambda'_{eo} (2\nabla (\nabla \cdot \mathbf{g}) - 2\Delta \mathbf{g} + 9D_4 (\nu \mathbf{u})), \tag{4.10}$$

where  $\Lambda'_{eo}$  denotes the  $\nu$  derivative of  $\Lambda_{eo}$

$$\Lambda_{eo} = \Lambda_e \Lambda_o = 3 \frac{\hat{T}}{\hat{L}^2} \Lambda_o \nu.$$

In the case  $\lambda^+ = \lambda^-$  where the TRT collision operator reduces to the BGK situation, the derivative is

$$\Lambda'_{eo} = 18 \frac{\hat{T}^2}{\hat{L}^4} \nu,$$

and does not vanish. Consequently, the equations

$$\nabla \cdot \mathbf{w}'_2 = 0, \quad \frac{1}{\varrho} \nabla p'_2 = \Delta \mathbf{w}'_2 + \frac{\partial}{\partial \nu} \bar{R}_0, \tag{4.11}$$



for the  $\nu$ -derivatives  $p'_2, w'_2$  of  $p_2, w_2$  has a source which, in general, does not vanish and thus leads to non-zero derivatives. In other words, a necessary condition for the invariance is  $\Lambda'_{e0} = 0$  which fixes the parameter  $\lambda^-$  completely. It has to be chosen as a function of  $\nu$  in such a way that  $\Lambda_{e0}$  is constant with respect to  $\nu$ . In this case, also the boundary condition for  $w_2$

$$w_2 \cdot c_i = \nu \Lambda_o \frac{\hat{L}}{3} (c_i \cdot \nabla) \frac{3\bar{u}}{\bar{p}} p - \hat{L}^2 \left( \Lambda_{e0} - \frac{1}{8} \right) (c_i \cdot \nabla)^2 (\nu u) \cdot c_i - \hat{T} \nu \Lambda_o g \cdot c_i,$$

is independent of  $\nu$  because

$$\nu \Lambda_o = \frac{3\hat{L}^2 \Lambda_{e0}}{\hat{T}},$$

so that  $w'_2 = 0$  on  $\partial\Omega$ . Choosing the particular value  $\Lambda_{e0} = 1/8$  has, in the case of bounce back algorithm with  $q_{ji} = 1/2$ , the additional advantage, that the cubic term in  $c_i$  vanishes, which has a regularizing effect.

The argument that  $\Lambda'_{e0} = 0$  is not only a necessary but also a sufficient condition for the  $\nu$ -independence, is outlined in [6].

We conclude this section with a remark on the role of the post-processing described in section 3.2.7. If, instead of (3.54), we had selected the definition (3.51), the source term would have contained an expression  $\hat{T}/2\nu\Delta g$  and  $\hat{T}/2\nu g \cdot c_i$  would have been found in the boundary condition for  $w_2$ . Both these terms are explicitly depending on  $\nu$  so that the considered invariance is not possible with definition (3.51), regardless of the choice of  $\lambda^-$ .

### 4.2 Instationary Stokes equation

Next, we focus on the invariance of the instationary Stokes equation

$$\partial_t u + \frac{1}{\varrho} \nabla p = \nu \Delta u + g, \quad \nabla \cdot u = 0,$$

discussed in section 2.1. For given  $\nu > 0$ , we pose the Stokes equation on the domain  $[0, T_\nu] \times \Omega$  with  $T_\nu = C/\nu$  and zero initial and boundary data for  $u$ . The source term  $g(t, x) = \eta(t/T_\nu, x)$  is defined in terms of a function  $\eta$  on  $[0, 1] \times \Omega$ . Then, the scaled versions of the solution  $p, u$

$$v(\tau, x) = \nu u(T_\nu \tau, x), \quad q(\tau, x) = p(T_\nu \tau, x),$$

are independent of  $\nu$ . In order to formulate a canonical discrete counterpart of

$$\frac{\partial}{\partial \nu} v = 0, \quad \frac{\partial}{\partial \nu} q = 0,$$

we have to make sure that the numerical solutions for different values of  $\nu$  are available at corresponding time points. The easiest way to achieve this is to choose  $T = T_\nu$

in the definition of the time step. Then  $\Delta t = T_v h^2$  is scaled to  $\Delta \tau = \Delta t / T_v = h^2$  so that the numerical solutions corresponding to various  $\nu$  can be compared at each point in time. According to the definition of  $\nu$ , we see that

$$\Lambda_e = 3\nu \frac{\Delta t}{\Delta x^2} = 3\nu \frac{T_v}{\hat{L}^2} = \frac{3C}{\hat{L}^2},$$

is independent of  $\nu$ . Also, the values of the source term  $g(t_k, x_j)$  entering the algorithm are identical in this case because

$$g(t_k, x_j) = \eta \left( \frac{k\Delta t}{T_v}, j\Delta x \right) = \eta(kh^2, j\Delta x).$$

If also  $\Lambda_o$  is chosen independently of  $\nu$ , the lattice Boltzmann algorithm is identical for each choice of  $\nu$  which carries over to the numerical solution. Hence, for  $T = T_v$ , the lattice Boltzmann algorithm possesses the invariance property.

Also in cases where the time step is chosen independently of  $\nu$ , the numerical solutions may still be comparable at certain subsets of the time points. For example, when  $\nu_1 = 5\nu_2$ , the scaled solutions corresponding to  $\nu_1$  and  $\nu_2$  are available at  $k\Delta t / T_{\nu_1}$  respectively  $l\Delta t / T_{\nu_2}$  with the relation

$$\frac{k\Delta t}{T_{\nu_1}} = \frac{5k\Delta t}{T_{\nu_2}} = \frac{l\Delta t}{T_{\nu_2}}, \quad l = 5k.$$

Thus, the solutions can be compared at every fifth point in time. To check the invariance in such cases, we investigate the  $(u_2, p_2)$ -equation. Applying the scaling to  $\hat{u}, \hat{p}$  amounts to the transformation

$$v_2(\tau, x) = \nu u_2(T_v \tau, x), \quad q_2(\tau, x) = p_2(T_v \tau, x),$$

of the expansion coefficients. Using Eq. (4.1), we find

$$\begin{aligned} \nabla \cdot v_2 + \frac{3C\hat{T}^2}{\varrho\hat{L}^2} \partial_\tau q &= 0, \\ \frac{1}{C} \partial_\tau v_2 + \frac{1}{\varrho} \nabla q_2 &= \Delta v_2 + \bar{R}_t + \bar{R}_0, \end{aligned}$$

with homogeneous initial conditions (if we had not set  $g(0, x) = 0$ , the initial value of  $v_2$  would be  $\nu\hat{T}/2\eta(0, x)$  leading to a loss of  $\nu$ -invariance already at this point). Since the source term  $\bar{R}_0$  does not contain time derivatives, it has exactly the same structure as in the stationary case. In particular, it is independent of  $\nu$  provided  $\Lambda'_{eo} = 0$ . Turning to the contribution  $\bar{R}_t$  defined in (4.3), we find

$$\bar{R}_t = -\frac{\Lambda_e \hat{T}}{T_v^2 \nu} \partial_\tau^2 v + \frac{2\hat{L}^2 \Lambda_{eo}}{3\nu T_v} \partial_\tau (\Delta v) + \frac{\hat{T}}{T_v} (\Lambda_e + 2\Lambda_o + 1) \partial_\tau \eta - \frac{6\nu \hat{T}^2}{\varrho \hat{L}^2 T_v} \partial_\tau \nabla q.$$

Since

$$\frac{\Lambda_e \hat{T}}{T_v^2 \nu} = \frac{3}{\hat{L}^2} \frac{\hat{T}^2}{T_v^2} = \frac{3\hat{T}^2}{\hat{L}^2 C^2} \nu^2,$$

we see that invariance is inevitably lost if  $\nu$  has a non-trivial time dependence. Moreover, time dependent sources lead to

$$\frac{\hat{T}}{C} (\nu \Lambda_e + 2\nu \Lambda_o + \nu) \partial_\tau \eta,$$

where only  $\nu \Lambda_o$  is  $\nu$ -independent if  $\Lambda'_{eo} = 0$ . We conclude that the  $\nu$ -independent behavior of the instationary Stokes solution can only be recovered by setting  $T = T_v$  in the algorithm. Otherwise, the independence is generally lost in contrast to the stationary case.

### 4.3 Navier-Stokes equation

Finally, we consider the classical scaling invariance of the Navier-Stokes equation discussed in section 2.1.5. For given Reynolds and Froude numbers, we choose  $L, T, \bar{p} > 0$  arbitrarily and define  $\bar{u}, \bar{g}, \rho, \nu$  as in (2.6). In this way, the full parameter vector  $\pi$  ranges over all of  $\Pi_{Re, Fr}$ .

With the source and boundary value defined as

$$\mathbf{u}_{bc}(t, \mathbf{x}) = \bar{u} \boldsymbol{\phi} \left( \frac{t}{T}, \frac{\mathbf{x}}{L} \right), \quad \mathbf{g}(t, \mathbf{x}) = \bar{g} \boldsymbol{\eta} \left( \frac{t}{T}, \frac{\mathbf{x}}{L} \right),$$

the scaled solution

$$\mathbf{v}(\tau, \mathbf{y}) = \bar{u}^{-1} \mathbf{u}(T\tau, L\mathbf{y}), \quad q(\tau, \mathbf{y}) = \bar{p}^{-1} p(T\tau, L\mathbf{y}), \tag{4.12}$$

is then independent of  $L, T, \bar{p}$ . Again, this behavior is exactly recovered for the numerical solution if we choose  $\hat{T} = T$  and  $\hat{L} = L$ . Then, we find

$$\Lambda_e = \frac{3\nu\hat{T}}{\hat{L}^2} = \frac{3}{Re'}, \quad \frac{\Delta t^2}{\Delta x} \mathbf{g} = \frac{h^3}{Fr} \boldsymbol{\eta}, \quad \frac{\Delta t}{\Delta x} \mathbf{u}_{bc} = h \boldsymbol{\phi},$$

and, as a consequence, the lattice Boltzmann algorithm is independent of  $T, L$  which, of course, carries over to the numerical solution. Moreover, the  $\rho$ -dependence is very simple because  $\hat{F}_i = \hat{f}_i / \rho$  is, by construction of the algorithm, independent of  $\rho$ . Observing that  $\hat{\mathbf{u}}$  is actually computed as velocity moment of  $\hat{F}_i$  because of the division by  $\rho$  in (3.54),  $\hat{\mathbf{u}}$  is independent of  $L, T$  and  $\rho$  and therefore independent of  $\bar{p} = \rho(L/T)^2$ . Similarly, the scaled pressure  $\hat{q} = \hat{p} / \bar{p}$  can be seen as computed from the average of  $\hat{F}_i$  because  $\rho^{-1}$  is introduced when dividing by  $\bar{p}$ . Altogether, the numerical solution possesses the full invariance in this case.

However, if we do not couple the space and time steps to the scaling parameters, the situation is quite different. As discussed in the previous example, a comparison

of two numerical solutions obtained with the same discretization parameters on differently scaled domains  $[0, T_1] \times L_1 \cdot \Omega^*$  and  $[0, T_2] \times L_2 \cdot \Omega^*$  is still meaningful on a subset of the spatial and temporal grid points if  $T_1, T_2$  and  $L_1, L_2$  are commensurable, i.e.  $m_1 T_1 = m_2 T_2$  and  $n_1 L_1 = n_2 L_2$  with  $M_i, n_i \in \mathbb{N}$ . Whether scaling invariance is possible in such cases can again be checked by considering the  $(\mathbf{u}_2, p_2)$ -equation.

Subjecting the numerical solution to the scaling described in (4.12) leads to a transformation of  $\mathbf{u}_2, p_2$  into

$$\mathbf{v}_2(\tau, \mathbf{y}) = \bar{u}^{-1} \mathbf{u}_2(T\tau, L\mathbf{y}), \quad q_2(\tau, \mathbf{y}) = \bar{p}^{-1} p_2(T\tau, L\mathbf{y}),$$

which satisfy the equations

$$\nabla_y \cdot \mathbf{v}_2 + \frac{3\bar{u}^2 \hat{T}^2}{\hat{L}^2} \partial_\tau q = 0, \tag{4.13a}$$

$$\partial_\tau \mathbf{v}_2 + \nabla_y p_2 + (\mathbf{v} \cdot \nabla_y) \mathbf{v}_2 + (\mathbf{v}_2 \cdot \nabla_y) \mathbf{v} = \frac{1}{Re} \Delta_y \mathbf{v}_2 + \hat{R}_t + \hat{R}_0. \tag{4.13b}$$

Already in the divergence condition, we see a  $\bar{u}$  dependence so that the solution varies, in general, with  $T$  and  $L$  unless the pressure is constant in time. Additional terms with lack of invariance are detected in the source term

$$\hat{R}_t = -\frac{3\nu \hat{T}^2}{\hat{L}^2 T} \partial_\tau^2 \mathbf{v}_1 + \frac{2 \hat{L}^2}{3 L^2} \Lambda_{eo} \partial_\tau (\Delta \mathbf{v}_1) + \frac{\hat{T}}{TFr} (\Lambda_e + 2\Lambda_o + 1) \partial_\tau \boldsymbol{\eta} - 6 \frac{\hat{T}^2 (\bar{U})^2}{\hat{L}^2 Re} \partial_\tau \nabla q_2,$$

and in the boundary condition where

$$-\frac{\hat{T}}{2T} \partial_\tau \boldsymbol{\phi} \cdot \mathbf{c}_i,$$

appears. Unless the boundary values  $\boldsymbol{\phi}$  are constant in time, this term acts like a non-homogeneous boundary value for  $\partial_\tau \mathbf{v}_2$  which, also due to sources in the governing equation, turns out to be nonzero.

We continue our investigation with the stationary case where  $\hat{R}_t = 0$  and the source is given by

$$\begin{aligned} \hat{R}_0 = & \frac{1}{12} \frac{\hat{L}^2}{L^2} \frac{1}{Fr} (1 - 8\Lambda_{eo}) \Delta_y \boldsymbol{\eta} + \frac{2}{3} \Lambda_{eo} \frac{\hat{L}^2}{L^2} \frac{1}{Fr} \nabla_y (\nabla_y \cdot \boldsymbol{\eta}) - \frac{1}{12 Re} \frac{\hat{L}^2}{L^2} \Delta_y^2 \mathbf{v} \\ & + \frac{3}{Re} \frac{\hat{L}^2}{L^2} (\Lambda_{eo} - \frac{1}{6}) D_{4,y}(\mathbf{v}) - \frac{\hat{L}^2}{L^2} (\Lambda_{eo} - \frac{1}{12}) D_{3,y}(\mathbf{v}, \mathbf{v}). \end{aligned} \tag{4.14}$$

While independence of  $T$  and  $\bar{p}$  is given when  $\Lambda'_{eo} = 0$  (here the definition of the force term (3.13) is crucial), an explicit  $L$ -dependence is still present so that invariance is lost. However, if we fix  $L$  and vary only  $T$  and  $\bar{p}$ , the boundary condition

$$\begin{aligned} \mathbf{v}_2 \cdot \mathbf{c}_i = & \frac{\Lambda_{eo} \hat{L}^2}{9 L^2} (\mathbf{c}_i \cdot \nabla_y) [3q + E_i(\mathbf{v}, \mathbf{v}, \varrho)] \\ & - \frac{\hat{L}^2}{L^2} (\Lambda_{eo} - \frac{1}{8}) (\mathbf{c}_i \cdot \nabla_y)^2 \mathbf{v} \cdot \mathbf{c}_i - \frac{\hat{L}^2}{L^2} \frac{\Lambda_{eo}}{3} \frac{Re}{Fr} \boldsymbol{\eta} \cdot \mathbf{c}_i, \end{aligned}$$

does not change so that the numerical solution may at least have a partial invariance in the case of stationary solutions with adapted space discretization  $\hat{L} = L$  which is supported by the direct analysis of the scheme in [6].

## 5 Conclusions

In this paper, we have used the detailed asymptotic analysis to investigate invariance properties of a TRT lattice Boltzmann algorithm. Generally, one can say that the basic scaling invariances are obeyed by the algorithm if the grid is scaled in the same way as the domain because the LB algorithm itself is easily seen to be invariant in this case.

However, when the same discretization parameters are used on differently scaled domains, the situation is different. Then, only the stationary case may show an invariance provided the free relaxation parameter  $\lambda^-$  is suitably defined (and if the spatial discretization is adapted to the scaling in the Navier-Stokes case). The stationary situation is carefully investigated in [6] on a discrete level containing much more information than our investigations which are only based on the equations of the leading order error contribution. As we have pointed out in section 2.2, expansion methods can only yield necessary conditions for invariance so that their strength is in showing that invariances are violated and not in proving invariance.

This has been demonstrated in the case of instationary problems. The analysis clearly shows that the invariance is lost at various points in the algorithm. For example, the initialization poses problems unless  $\mathbf{g}(0, \mathbf{x}) = 0$  and the boundary condition violates invariance if  $\phi$  is not constant in time. Finally, the time derivatives of the Stokes or Navier-Stokes solutions act as sources with lacking invariance in the governing equation of the leading order error.

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