

Grad's approximation for moving and stationary walls in entropic lattice Boltzmann simulations

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ABSTRACT

We introduce a new generalized wall boundary condition for the entropic lattice Boltzmann method (ELBM) that is capable of handling complex flow geometries including moving walls. The Grad's ten moments approximation is employed to approximate the missing populations at the boundary nodes. The new boundary condition significantly improves accuracy, stability and sub-grid features of LBM and in particular of its entropic variant, ELBM. The proposed boundary condition is tested for a range of flows in two dimensions, including planar channel flow, Couette flow, flow past a circular cylinder and sedimenting circular particles. Further simulations involving complex geometries such as flapping wing and transversely oscillating cylinder demonstrate superior stability and accuracy of the new wall boundary condition.

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1. Introduction

Accurate simulations of moving objects with complex geometries in fluid flows is of great interest in numerous fields such as biomedical flows, animal locomotion and also various industrial applications. To that end, we use the lattice Boltzmann method (LBM) as it has evolved into an accurate and efficient alternative to the conventional computational fluid dynamics. The lattice Boltzmann method has its origin in the kinetic theory and describes the flow field in terms of the dynamics of discretized particle distribution functions, as opposed to a direct discretization of the Navier–Stokes equation, see e.g., the pioneering work of Benzi et al. [1] or the book of Succi [2]. Nevertheless, by using Chapman–Enskog analysis, one can show that the macroscopic Navier–Stokes equation can be recovered in the hydrodynamic limit (see, e.g., Chapman and Cowling [3], Ansumali and Karlin [4], Qian et al. [5], Shan and He [6]). Apart from the classical Bhatnagar–Gross–Krook lattice Boltzmann model (LBGK), several other variants have been developed. Most notable is the entropic lattice Boltzmann method (ELBM), which was started off by Karlin et al. [7,8] and Succi et al. [9], as it distinguishes itself from other models by the fact that it obeys the second law of thermodynamics using the discrete-time H-theorem, yielding a local, self-adaptive, parameter-free and unconditionally stable discretization. Thus, the ELBM opened the door for turbulent flow simulations at high Reynolds numbers without the need for explicit sub-grid models, while recovering the conventional LBGK approximation in the limiting case of low Reynolds numbers and resolved grid.

For the treatment of generic, curved walls, there are two main approaches available in the context of LBM, namely immersed boundary methods and Cartesian grid approaches. The immersed boundary method (IBM), first proposed by

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Peskin [10], treats the boundary as deformable and introduces a set of Lagrangian points to represent the boundary independently from the underlying Eulerian mesh needed by the LBM. A deformation or motion of the boundary yields a force that tends to restore the boundary to its initial state. The fluid-structure interaction is then realized by a smooth distribution of the restoring force among the neighboring grid points, thus coupling the Eulerian and the Lagrangian mesh. The main issue in IBM is the computation of the restoring force. Based on the work of Peskin [10], several derivatives have been developed, adopting different computational methods of the force. Among others, there are penalty methods [10], direct forcing methods [11] and momentum exchange methods [12]. Note that these schemes do not enforce the no-slip condition exactly, which may lead to streamlines penetrating the solid object. A notable exception is the velocity-correction method as proposed by Wu and Shu [13] involving an implicit computation of the restoring force.

In the context of Cartesian grid methods, various boundary conditions for generic, curved walls can be found in the lattice Boltzmann literature, but most commonly interpolation or extrapolation schemes are employed on the particle distribution to compensate the crude staircase approximation of the geometry by the underlying uniformly spaced grid of the LBM. A popular representative of such kind is the interpolated bounce back boundary condition (IBB) as presented in the article of Lallemand and Luo [14]. In this context, an extension to moving boundaries was proposed by introducing a force expressed in terms of the populations in order to account for the momentum exerted from the boundary onto the fluid. However, due to the highly fluctuant nature of the populations, interpolation or extrapolation schemes are prone to numerical instabilities. As a consequence, in the simulation of wall-bounded turbulent flows using boundary conditions of such kind, one can observe discontinuities or shocks, triggered at the boundary, propagating into the bulk (see, e.g., Lammers et al. [15], Spasov et al. [16]). This issue was partially resolved for stationary walls by the so-called Tamm–Mott–Smith (TMS) boundary condition as proposed by Chikatamarla and Karlin [17]. However, a universal approach for generic, moving wall boundaries has not been developed for the ELBM.

For this purpose, a novel treatment of complex, non-stationary wall boundaries is proposed below, which is similar in spirit to the IBM but is imposed on the density and velocity fields directly. The idea of the scheme in this paper is to impose the boundary condition not directly on the populations itself but in terms of the inherently smoother macroscopic quantities such as density and momentum by employing an analog of Grad's approximation. In the context of kinetic theory, a discussion of Grad's approximation can be found in, e.g., Gorban and Karlin [18]. It is noted that the proposed boundary condition is, in a way, an extension of a similar treatment of "missing populations" first proposed by Chikatamarla et al. [19] for the outflow boundary condition. Due to its evaluation on the Cartesian grid the common issues arising from the computation and distribution of the restoring force in the context of IBM are eliminated. Thus, the stability issues are resolved while accuracy and simplicity are not compromised. Note, a comparative study of IBB as a Cartesian grid method and IBM can be found in the article of Peng and Luo [20], which highlights the superiority of Cartesian grid methods in terms of accuracy and consequently efficiency in the LB context.

The remainder of this paper is organized as follows. Section 2 gives an overview of the numerical methodology, starting with a brief description of the entropic lattice Boltzmann scheme and followed by the derivation of the proposed boundary condition. For validation, various benchmark simulations are presented in section 3. First, the simple case of a flow past a two-dimensional, stationary, circular cylinder is simulated in order to access the accuracy and stability for curved boundaries without the additional complication of a non-stationary wall. As a second step, simulations of moving objects such as a transversely oscillating cylinder, a sedimenting circular particle and a flapping wing are presented and compared to data from the literature. In Section 4, the results are summarized and conclusions are drawn.

2. Numerical methodology

2.1. Entropic lattice Boltzmann method

With its origin in the kinetic theory, the lattice Boltzmann method describes the fluid state in terms of populations $f_i(\mathbf{x}, t)$ associated with a set of discrete velocities $\mathbf{c}_i$. The evolution of the populations is described by the discrete kinetic equation

$$f_i(\mathbf{x} + \mathbf{c}_i, t + 1) - f_i(\mathbf{x}, t) = \Omega_i, \quad (1)$$

consisting of an advection step along the discrete velocities $\mathbf{c}_i$ and a relaxation step represented by the collision operator Ω_i . The fluid density ρ and the momentum $\mathbf{j} = \rho \mathbf{u}$ are defined as the first two moments of the distribution function, which are given by

$$\rho = \sum_i f_i, \quad \mathbf{j} = \sum_i \mathbf{c}_i f_i. \quad (2)$$

In the case of the entropic lattice Boltzmann model as derived in Karlin et al. [7,8] and Succi et al. [9], the collision operator is written as

$$\Omega_i = \alpha \beta (f_i^{eq} - f_i), \quad (3)$$

where the local equilibrium function f_i^{eq} is defined as the minimum of the discrete entropy function H (entropy = $-H$) subject to the local conservation laws

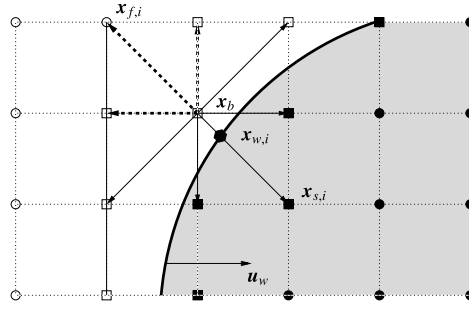


Fig. 1. The unknown populations at the boundary are represented as the dashed arrows. ●: Solid nodes. ○: Fluid nodes. ■: Solid boundary nodes. □: Fluid boundary nodes.

$$\min \left\{ H(f) = \sum_i f_i \ln \left(\frac{f_i}{W_i} \right) \right\} \quad \text{s.t.} \quad \sum_i \{1, \mathbf{c}_i\} f_i = \{\rho, \mathbf{j}\} \quad (4)$$

with the lattice weights W_i specific to a given velocity set. The relaxation parameter is split into two parts, the maximal over-relaxation α and the parameter β , which is linked to the kinematic viscosity. The entropic over-relaxation α is found as the positive root of the entropy condition

$$H(f + \alpha(f^{eq} - f)) = H(f), \quad (5)$$

thus ensuring the time-discrete H-theorem for which the total entropy $\hat{H}(t) = \sum_{\mathbf{x}} H(f(\mathbf{x}, t))$ is not increasing in time for any given $\beta \in [0, 1]$. For a sufficient grid resolution, the populations stay close to the local equilibrium and the maximal over-relaxation is automatically computed as $\alpha = 2$. Hence, for resolved simulations, the ELBM results in the well-known LBGK model, which recovers the Navier–Stokes equation in the hydrodynamic limit with the kinematic viscosity

$$\nu = c_s^2 \left(\frac{1}{2\beta} - \frac{1}{2} \right), \quad (6)$$

and the lattice speed of sound $c_s = 1/\sqrt{3}$ for standard lattices. However, in order to prevent numerical instabilities, the ELBM scheme adapts the over-relaxation parameter in accord with the time-discrete H-theorem, yielding a parameter free and non-linearly stable numerical scheme. We compute α at each grid point and time step using a Newton–Raphson (NR) scheme with a tolerance of 10^{-5} for convergence of α . In practice, the NR scheme takes on average 3 to 4 iteration to converge. When the NR scheme does not find a solution in 15 iterations, we use the LBGK over-relaxation $\alpha = 2$.

For our simulations, we consider the two-dimensional ELBM on a nine velocity lattice, D2Q9. In this case, the velocity set is given as

$$\mathbf{c}_i = \begin{cases} (0, 0), & i = 0 \\ (\cos[(i-1)\pi/2], \sin[(i-1)\pi/2]), & i = 1-4 \\ (\cos[(i-1)\pi/2 + \pi/4], \sin[(i-1)\pi/2 + \pi/4])\sqrt{2}, & i = 5-8. \end{cases} \quad (7)$$

As shown in the article of Ansumali et al. [21], the explicit solution of the minimization problem in Eq. (4) yields the equilibrium distribution function

$$f_i^{eq} = \rho W_i \prod_{j=1}^{D=2} \left(2 - \sqrt{1 + 3u_j^2} \right) \left(\frac{2u_j + \sqrt{1 + 3u_j^2}}{1 - u_j} \right)^{c_{ij}}, \quad i = 0, 1, \dots, 8 \quad (8)$$

with the lattice weights

$$W_i = \begin{cases} 4/9, & i = 0 \\ 1/9, & i = 1-4 \\ 1/36, & i = 5-8. \end{cases} \quad (9)$$

2.2. Grad's approximation for curved and moving wall boundaries

For the treatment of moving boundaries, let us consider Fig. 1. For the general boundary node $\mathbf{x}_b$ in the fluid domain, populations $f_i(\mathbf{x}_b, t)$, belonging to the subset $\bar{D}$ of velocities pointing from the solid into the fluid domain, are unknown and must be specified in order to complete the advection step of the ELBM scheme. Those “missing” populations are indicated by the dashed arrows in Fig. 1. To specify the missing populations $f_i(\mathbf{x}_b, t)$ for $i \in \bar{D}$, a similar approach as in the article

of Chikatamarla et al. [19] is taken, where an analog of Grad's moment approximation for the distribution functions is introduced. Originally, Grad's moment approximation stems from a truncated expansion in the Hermite velocity polynomials around the local Maxwellian. The resulting distributions are parametrized by the moment system, where not only locally conserved quantities but also the stress tensor and the energy flux are taken into account. However, it has been shown that by quasi-equilibrium considerations other higher-order moments may be included (see Gorban and Karlin [22,18]). In the case of an athermal flow, it is sufficient to include the locally conserved quantities ρ and $\mathbf{j}$ as well as the pressure tensor $\mathbf{P}$. The approximation of the population can now be written as

$$f_i^*(\rho, \mathbf{j}, \mathbf{P}) = W_i \left[\rho + \frac{\mathbf{j}_\alpha c_{i\alpha}}{c_s^2} + \frac{1}{2c_s^4} (P_{\alpha\beta} - \rho c_s^2 \delta_{\alpha\beta}) (c_{i\alpha} c_{i\beta} - c_s^2 \delta_{\alpha\beta}) \right]. \quad (10)$$

As suggested by the standard multi-scale Chapman–Enskog analysis, the pressure tensor is well approximated by the first two terms of its power-series expansion as

$$P_{\alpha\beta} = P_{\alpha\beta}^{eq} + P_{\alpha\beta}^{neq} \quad (11)$$

with the equilibrium and non-equilibrium parts

$$P_{\alpha\beta}^{eq} = \rho c_s^2 \delta_{\alpha\beta} + \rho u_\alpha u_\beta, \quad (12)$$

$$P_{\alpha\beta}^{neq} = -\frac{\rho c_s^2}{2\beta} \left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha} \right), \quad (13)$$

where the later is evaluated using a first-order finite difference scheme and the velocities given from the previous time step. The boundary condition is therefore not local anymore but accesses additional information from the neighboring cells in order to compute the velocity gradients. As shown by Latt et al. [23], this additional information is crucial in terms of accuracy. Furthermore, we propose to evaluate Eq. (10) for the unknown populations by using specified target values $\mathbf{u}_{tgt}$ and ρ_{tgt} to account for curved as well as moving boundaries. The target velocity $\mathbf{u}_{tgt}$ at a given boundary node $\mathbf{x}_b$ may be obtained by an interpolation scheme involving the wall velocity $\mathbf{u}_{w,i} = \mathbf{u}(\mathbf{x}_{w,i}, t)$ at the intersection point $\mathbf{x}_{w,i}$ and the velocities $\mathbf{u}_{f,i} = \mathbf{u}(\mathbf{x}_{f,i}, t)$ at the adjacent fluid nodes $\mathbf{x}_{f,i} = \mathbf{x}_b + \mathbf{c}_i$ for $i \in \bar{D}$ (see Fig. 1). For an averaged linear interpolation, this yields

$$\mathbf{u}_{tgt} = \frac{1}{n_{\bar{D}}} \sum_{i \in \bar{D}} \frac{q_i \mathbf{u}_{f,i} + \mathbf{u}_{w,i}}{1 + q_i}, \quad (14)$$

where $n_{\bar{D}}$ is the number of unknown populations. The parameter q_i is the fluid fraction of the corresponding grid spacing, which is defined through the intersection point $\mathbf{x}_{w,i}$ of the boundary along the direction $\mathbf{c}_i$ as $q_i = \|\mathbf{x}_b - \mathbf{x}_{w,i}\| / \|\mathbf{c}_i\|$. This ensures correct wall velocity as well as it accounts for the momentum exerted from a moving object onto the fluid. In order to assign a value for ρ , which is a pseudonym for the pressure in LB simulations of quasi-incompressible flows ($p = \rho c_s^2$), the target density ρ_{tgt} is set to be

$$\rho_{tgt} = \rho_{bb} + \rho_s \quad (15)$$

with

$$\rho_{bb} = \sum_{i \in \bar{D}} f_i^{bb} + \sum_{i \notin \bar{D}} f_i, \quad (16)$$

$$\rho_s = \sum_{i \in \bar{D}} 6W_i \rho_0 \mathbf{c}_i \cdot \mathbf{u}_{w,i}, \quad (17)$$

where the first term ρ_{bb} denotes the density implied by the standard bounce back boundary condition for which the unknown distribution functions are replaced by the reflected populations as $f_i^{bb} = \tilde{f}_i$ with $\tilde{\mathbf{c}}_i = -\mathbf{c}_i$. The second contribution ρ_s accounts for the local density alteration caused by the mass displacement, occurring as the object is moving with the velocity $\mathbf{u}_w$. It can be derived by introducing a forcing term F_i , which is necessary for the displacement. Following the derivation given by Luo [24,25] for the D2Q9 lattice, the conservation of mass and momentum

$$\sum_i F_i = 0, \quad (18)$$

$$\sum_i \mathbf{c}_i F_i = \rho_0 \mathbf{u}_w \quad (19)$$

lead to

$$F_i = 6W_i \rho_0 \mathbf{c}_i \cdot \mathbf{u}_w. \quad (20)$$

Finally, the summation of the forcing term over all populations in $\bar{D}$ can be interpreted as the density change caused by the displacement of mass. It is noted that a similar approach is presented in the article of Latt et al. [23] for the regularized

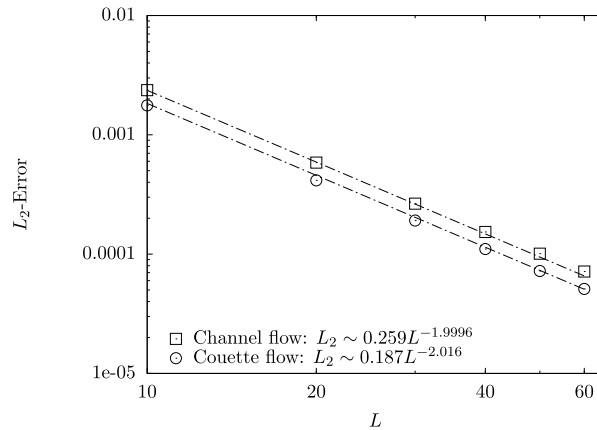


Fig. 2. Scaling of L_2 error for the simulation of channel flow and Couette flow at $Re = 100$.

boundary condition of a stationary straight wall using the local values for the density and the velocity. However, in contrast to Latt et al. [23] and in accordance with Chikatamarla et al. [19], we propose not to replace all populations, but only the unknown populations in order to keep the information of the surrounding fluid. Furthermore, the concept of the target values, as presented above, extends the boundary condition to curved and moving walls.

It is important to note that the proposed boundary condition does not impose the desired values of the macroscopic quantities exactly at the boundary (since only the missing populations are replaced). Hence, we need to investigate the effect of the boundary condition on the macroscopic quantities at the wall thoroughly. To this end, we simulate a channel flow to measure the velocity slip at the wall and the order of convergence of the boundary condition. Fig. 2 shows the scaling of the L_2 error of velocity with respect to the grid size for the simulation of channel flow (driven by body force) for a Reynolds number of $Re = 100$. As expected, second order convergence is clearly seen in this plot. The velocity slip at the wall was measured to be around 10^{-5} to 10^{-7} (depending on the grid resolution) in lattice units which is small compared to the flow velocity typically of the order of 10^{-2} (lattice units); hence this does neither affect the flow field far away nor close to the wall. To further investigate the order of convergence also for a non-stationary case involving moving walls, we consider the time evolution of the Couette flow for which the bottom plate moves with a constant velocity $\mathbf{u}_w$ whereas the top plate is at rest. Initially, the velocity is set to zero everywhere except on the top boundary. The L_2 error is computed for the initial transient phase till steady state is reached by comparison to its analytical solution (see, e.g., Muzychka and Yovanovich [26]). As it is apparent from Fig. 2, the proposed boundary condition recovers a second order of accuracy also for non-stationary walls. Furthermore, excellent agreement was found for the evaluation of drag and lift forces at the wall (see next section).

As indicated in Fig. 1, another aspect to consider in the context of moving boundaries is the reinitialization of the solid boundary nodes (filled squares), which move out of the solid region into the fluid domain as the object passes. Here, we use the equilibrium distribution functions with the wall velocity and the system averaged density. As stated in the article of Lallemand and Luo [14], there are different possibilities for the reinitialization. For instance, the unknown populations may be obtained by a second-order extrapolation or a consistent update of the populations in the solid region by performing collisions while the velocity is kept constant at the wall velocity. We confirm the results of Lallemand and Luo [14] that all choices produce similar results. Finally, it is noted that the wall-velocity may not be too large compared to the speed of sound c_s .

2.3. Force evaluation

A key parameter to validate our simulations is the force acting on a given object. Hence, the method to evaluate the forces will be briefly reviewed in this section. The total force acting on the object can be split into a pressure force and a part corresponding to the viscous shearing stresses, which leads to the expression

$$\mathbf{F} = \int_{\partial\Omega} dA \hat{\mathbf{n}} \left\{ -p \mathbf{I} + \rho \nu \left[(\nabla \mathbf{u}) + (\nabla \mathbf{u})^T \right] \right\}, \quad (21)$$

where $\hat{\mathbf{n}}$ denotes the outward normal vector of the object boundary $\partial\Omega$. The direct evaluation of the surface integral is not straightforward, since the values for the pressure and the deviatoric stresses need to be extrapolated onto the curved surface for an accurate computation. As an alternative, the force may be evaluated by means of the momentum-exchange method, where it is described through a summary of the momentum fluxes. Given a general boundary node located at $\mathbf{x}_b$ as in Fig. 1, the momentum exchange with the neighboring nodes in the solid region is given by

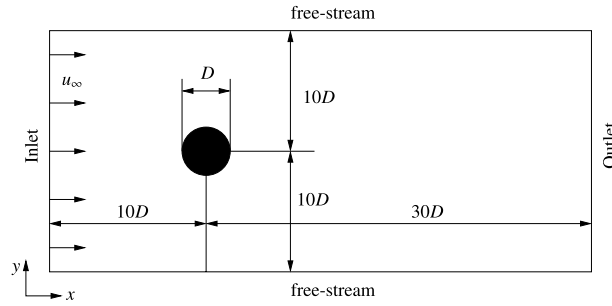


Fig. 3. Schematic of a flow past a circular cylinder.

$$\sum_{i \in \bar{D}} \tilde{\mathbf{c}}_i \left[f_i(\mathbf{x}_b, t) + \tilde{f}_i(\mathbf{x}_{s,i}, t) \right], \quad (22)$$

where $\mathbf{x}_{s,i} = \mathbf{x}_b + \tilde{\mathbf{c}}_i$ and $\tilde{f}_i$ is associated with the opposite velocity $\tilde{\mathbf{c}}_i = -\mathbf{c}_i$. The summation over all boundary nodes finally yields the total force

$$\mathbf{F} = \sum_{\text{all } \mathbf{x}_b} \sum_{i \in \bar{D}} \tilde{\mathbf{c}}_i \left[f_i(\mathbf{x}_b, t) + \tilde{f}_i(\mathbf{x}_{s,i}, t) \right]. \quad (23)$$

An extensive comparison between the direct evaluation of the surface integral and the momentum-exchange method was conducted by Mei et al. [27], showing the superiority of the momentum-exchange method in terms of efficiency, accuracy and robustness for curved boundaries. For this reason, we choose the momentum-exchange method to evaluate the force acting on a given object.

3. Results and discussion

In this section, various benchmark simulations are presented and compared to results found in the literature in order to access the accuracy and the stability of the proposed boundary condition. First, the case of a flow past a stationary, circular cylinder is considered, followed by the simulation of a transversely oscillating cylinder, a sedimenting circular particle and finally a flapping wing. For all simulations, the equilibrium distributions are used for the initial and the inlet boundary condition. At the outlet, the no-boundary condition is applied. A grid convergence study was done for all cases and only converged values are reported. Unless stated otherwise, all parameters are given in lattice units.

3.1. Flow past a stationary cylinder

In order to examine the ability of the proposed boundary condition to handle curved boundaries, the well studied case of a flow past a stationary, circular cylinder is considered. The resulting flow pattern behind the cylinder is highly dependent on the Reynolds number, which is defined in terms of the free-stream velocity u_∞ , the diameter D and the kinematic viscosity ν as $Re = u_\infty D / \nu$. For low Reynolds numbers $Re \leq 47$, the flow field converges towards a steady state solution, whereas an increase of the Reynolds number yields the unsteady wake pattern of the von Kármán vortex street. The von Kármán vortex street develops due to periodic detachment of vortices with opposite circulation from each side of the cylinder, forming a street of alternating vortices in the wake of the cylinder. Most commonly, the lift and the drag coefficients are used to characterize the flow field, which are defined by

$$C_D = \frac{F_D}{\frac{1}{2} \rho_\infty u_\infty^2 D}, \quad C_L = \frac{F_L}{\frac{1}{2} \rho_\infty u_\infty^2 D}, \quad (24)$$

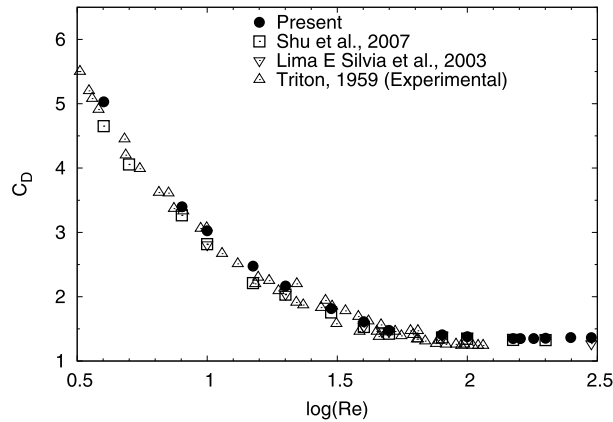
where F_D and F_L denote the force exerted onto the cylinder in the stream-wise and transverse direction with respect to the mean flow, respectively. The density in the free-stream is indicated by ρ_∞ and is generally taken to be unity. In addition, in the unsteady case, the Strouhal number St , corresponding to the non-dimensional vortex shedding frequency, is defined as

$$St = \frac{f_s D}{u_\infty}, \quad (25)$$

where f_s is the dominant shedding mode. As depicted in Fig. 3, the cylinder with a diameter of $D = 20$ is placed in a rectangular domain, where a uniform inlet condition with $u_\infty = 0.05$ as well as free-stream boundary conditions at the bottom and the top are applied. The free-stream boundary condition is typically realized by a reflection of the impinging populations with respect to the normal vector of the boundary. The domain dimensions were chosen sufficiently large

Table 1Comparison of the non-dimensional recirculation length $\tilde{L} = 2L/D$ for $Re = 20$ and $Re = 40$.

Reference	$Re = 20$	$Re = 40$
Dennis and Chang [28]	1.88	4.69
Nieuwstadt and Keller [29]	1.786	4.357
Coutanceau and Bouard [30]	1.86	4.26
Fornberg [31]	1.82	4.48
He and Doolen [32]	1.842	4.49
Niu et al. [12]	1.89	4.52
Shu et al. [33]	1.80	4.40
Present	1.85	4.50

**Fig. 4.** Comparison of the mean drag coefficient for the flow past a stationary circular cylinder at various Reynolds numbers.

to minimize the effect of the domain boundaries. In this section, both steady and unsteady cases are simulated. For an accelerated vortex formation in the unsteady flow regime a small, initial perturbation of the flow field was introduced.

First, as shown in Table 1, we consider the non-dimensional recirculation length $\tilde{L} = 2L/D$ for the Reynolds numbers $Re = 20$ and $Re = 40$ and compare it to values reported in previous studies. In this context, the recirculation length L is defined as the distance from the rearmost point of the cylinder to the end of the recirculating region. It is evident that our results match well with the values found in the literature. Second, Fig. 4 shows the dependency of the mean drag coefficient on the Reynolds number and the results are compared to the data obtained experimentally and numerically by Shu [33], Silva et al. [34] and Tritton [35]. The drag force F_D was computed using the momentum-exchange method as in Eq. (23). It is clear from Fig. 4 that our results are in good agreement with the reference data. For further validation of the unsteady flow regime, a comparison of the Strouhal number for different Reynolds numbers to the results reported by Norberg [36] and Williamson [37] is shown in Fig. 5. The Strouhal number is defined by means of the dominant vortex shedding frequency f_s , which is evaluated with the aid of a discrete Fourier transform of the velocity field measured at an off-center location downstream of the cylinder. As shown in Fig. 5, the results are consistent with the data published in literature. With a good agreement in both steady and unsteady cases, the proposed boundary condition has proven to be an accurate scheme for curved boundaries on a standard lattice Boltzmann grid.

Finally, we evaluate the stability limits of the boundary condition. For this purpose, the simulations are not stabilized through the entropic relaxation as in Eq. (5), but the classical LBGK model with $\alpha = 2$ is used. A gradual increase of the Reynolds number under the same conditions as described above yields a stability limit of $Re = 2200$ for the current boundary condition. For comparison, simulations using the interpolated bounce back boundary condition as in the article Lallemand and Luo [14] are stable only up to $Re \approx 200$.

3.2. Flow past a transversely oscillating cylinder

Having validated our simulations in the stationary case, the flow past a transversely oscillating cylinder at a fixed Reynolds number of $Re = 100$ is considered. This case is a both numerically and experimentally well studied problem and therefore a good benchmark for the proposed boundary condition. The simulations are compared to the numerical studies of Bao et al. [38] and Placzek et al. [39], which employ a multiple-relaxation-time lattice Boltzmann model and a finite volume Navier–Stokes solver, respectively. The setup is similar to the stationary case as shown in Section 3.1 except that the cylinder is forced to follow a periodic motion

$$y(t) = y_{\max} \sin(2\pi f_0 t), \quad (26)$$

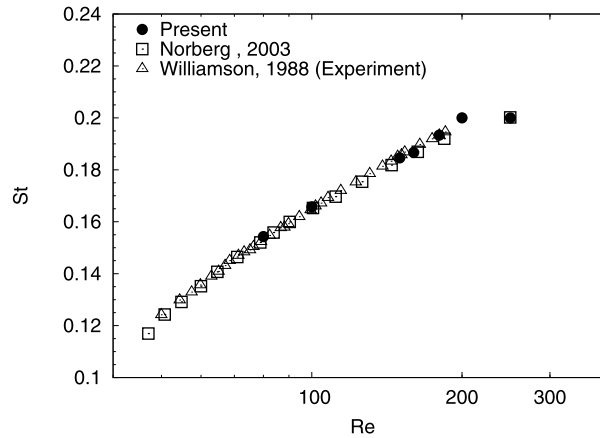


Fig. 5. Comparison of the Strouhal number for different Reynolds numbers.

which is characterized by its frequency f_0 and the non-dimensional amplitude $A = y_{\max}/D$, where $y_{\max}$ denotes the maximal vertical displacement. Although, the cylinder oscillates independent of the flow, the wake of the cylinder is strongly affected by its motion. Different regimes of the wake can be characterized using the non-dimensional amplitude A and a non-dimensional frequency $F = f_0/f_s$, where f_s is the natural vortex shedding frequency of a stationary cylinder at the same Reynolds number. In our case, the amplitude is kept constant at $A = 0.25$ and simulations for different frequency ratios F are carried out. This yields two main configurations, the so-called lock-in and the unlocked regime. For frequencies in the region between two almost symmetrical limits around $F = 1$, the vortex shedding frequency in the wake of the cylinder synchronizes with the imposed frequency f_0 . This phenomena is called the lock-in regime and the wake is purely sinusoidal and solely governed by the imposed frequency. Outside this region, the unlocked regime is observed, where both the natural frequency as well the imposed frequency contribute to the wake pattern. To study both regimes, we consider a wide frequency range of $F = 0.5$ – 1.5 . In Fig. 6, the evolution of the fluctuating lift coefficient C'_L along with its power spectrum and its phase diagram are shown for different frequencies. The lock-in region is exemplarily represented by the frequencies $F = 0.9$ and $F = 1.1$, where the time series of the fluctuating lift coefficient are in fact purely sinusoidal oscillations with the frequency f_0 . The natural shedding frequency f_s does not contribute to the oscillation. Accordingly, the power spectra show only one peak at $f^* = f/f_0 \approx 1$. The phase diagrams in the right column of Fig. 6 indicate the energy transfer between the cylinder and the fluid. For the lock-in frequencies $F = 0.9$ and $F = 1.1$, the phase diagrams are consistent with the history of the lift coefficient and the power spectrum, as they correspond to one unique cycle. The unlocked configurations are illustrated by the frequencies $F = 0.5$ and $F = 1.5$. The power spectra now exhibit two peaks, corresponding to the forced and the natural Strouhal frequency located at $f^* \approx 1$ and $f^* \approx 1/F$, respectively. The main frequency governs the cycle-to-cycle oscillation, while the minor frequency is associated to the signal periodicity. Therefore, in the case of $F = 0.5$, the main peak is at $f^* \approx 2$, which means that the cycle-to-cycle periodicity is given by the inverse of the Strouhal frequency, whereas the signal periodicity is determined through f_0 . For the frequency $F = 1.5$ it is reversed, since the main frequency now corresponds to the imposed and the less dominated to the Strouhal frequency. The existence of more than one frequency is also reflected by the shape of the phase diagrams, which now exhibit a much more irregular pattern compared to the locked configurations.

Having found a physically consistent behavior for the evolution of the lift coefficient, the mean drag and lift coefficient for different frequencies are now compared in Fig. 7 to the values found by Bao et al. [38] and Placzek et al. [39]. For the drag coefficient, all curves show the same global trend, where the maximum of the drag is located within the lock-in regime around $F = 1.1$. Similarly, the lift coefficient exhibits a steep increase in the lock-in region, which is again compensated when the unlocked regime is entered. The obtained curves match especially well with results of Placzek et al. [39]. As it was pointed out by Bao et al. [38], the discrepancy of their results to those of Placzek et al. [39] and our simulations arises from the fact that the drag coefficient for the stationary case differs as well. The mean drag in the stationary case yields $C_D = 1.353$ for Bao et al. [38], whereas Placzek et al. [39] report $C_D = 1.37$. As shown in Section 3.1, we obtain a mean drag of $C_D = 1.3778$ for the stationary case, which is why our results follow the ones from Placzek et al. [39] significantly closer.

Analogous to the case of the flow past the stationary cylinder, we also assess the stability limits in the present case for a moving boundary in a LBGK simulation. A similar behavior can be observed and stability is increased up to a Reynolds number of $Re = 2300$ as compared to the interpolated bounce back scheme which yields stability of up to $Re \approx 200$.

3.3. Sedimentation of a circular particle

In this section, the problem of the sedimentation of a circular particle under gravity in an infinite channel is considered. The problem has been studied extensively by Wang et al. [40] and is schematically described by Fig. 8. A circular particle

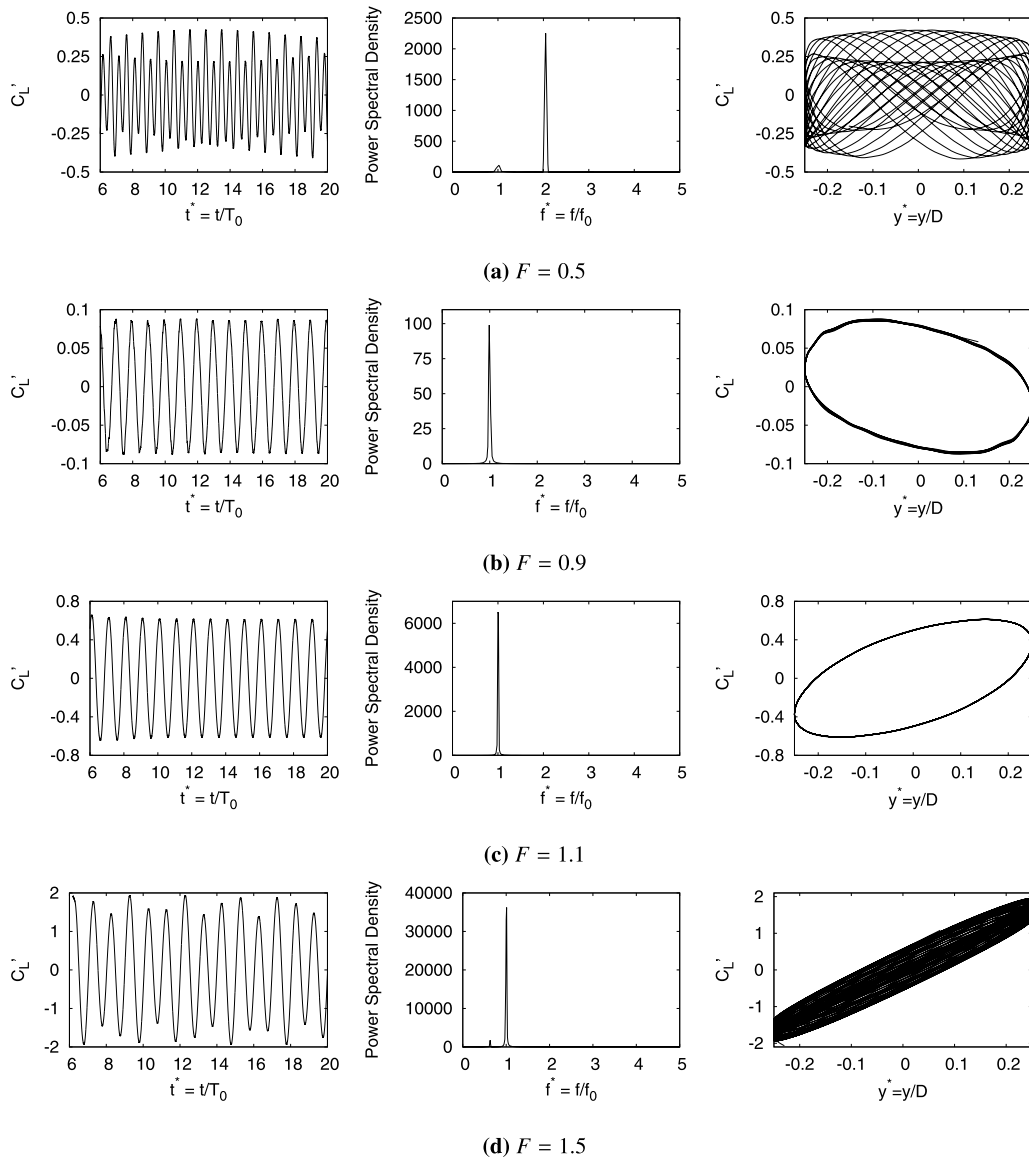


Fig. 6. The time history (left), the power spectrum (middle) and the phase portrait (right) of the fluctuating lift coefficient for selected frequencies.

of diameter D is placed in a channel of size $H \times W$, where the gravitational force is acting in negative y -direction. Initially, the particle is at rest and its motion is described by Newton's law

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{u}_p, \quad (27)$$

$$\frac{d\mathbf{u}_p}{dt} = \frac{\mathbf{F}}{m_p} + \left(1 - \frac{\rho_f}{\rho_p}\right) \mathbf{g}, \quad (28)$$

where $\mathbf{x}_p$, $\mathbf{u}_p$, m_p , ρ_p indicate the position, the velocity, the mass and the density of the particle, respectively. The total force acting on the particle as in Eq. (23) is denoted by $\mathbf{F}$ and the fluid density by ρ_f . Note that in the equations above and in contrast to e.g., Uhlmann [41] there is no explicit term to account for added mass. However, the added mass term is already implicitly contained in the boundary condition itself and is included in the target density by the contribution of ρ_s (see Eq. (17)). This is possible, because we introduce a force expressed in terms of the populations as in Eq. (20) and a summation over the force terms yields the local density alteration due to added mass. On the other hand, the momentum exerted onto the fluid is accounted for by using the corresponding target velocity for the computation of Grad's approximation for the population. Thus, the evolution equation of the particle reduces to a simple momentum balance as in Eq. (28).

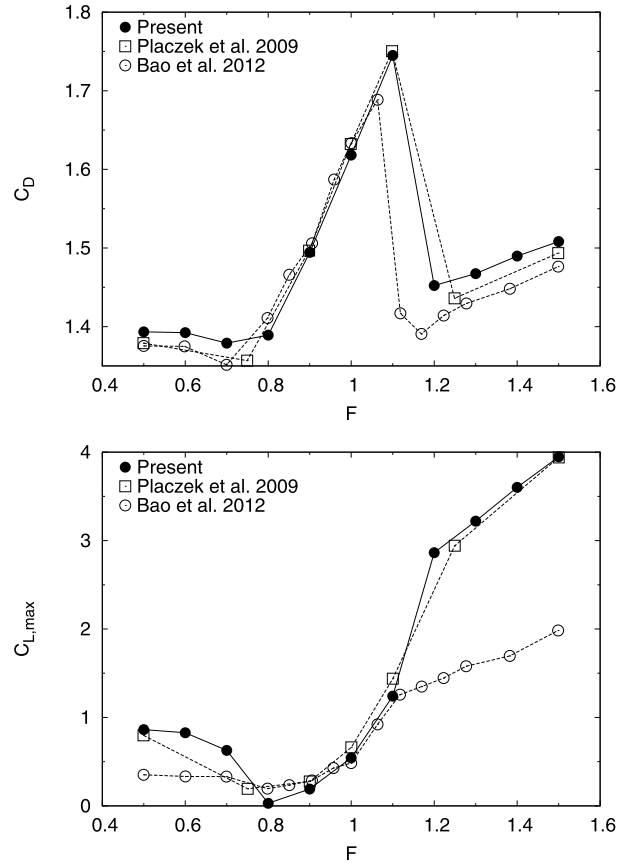


Fig. 7. The dependency of the mean drag and the maximal lift coefficient on the frequency.

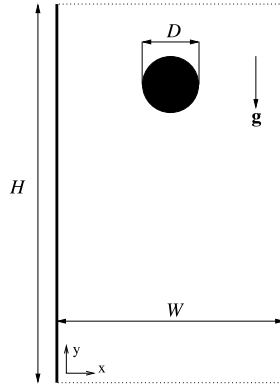


Fig. 8. Schematic of the sedimentation of a circular particle under gravity.

At low Reynolds numbers, there exists an approximate analytical solution proposed by Happel and Brenner [42], for which the drag force on a circular particle between two infinite plates may be approximated as

$$\mathbf{F}_d = 4\pi C \mu \mathbf{u}_s \quad (29)$$

with μ and $\mathbf{u}_s$ denoting the dynamic viscosity and the settling velocity of the particle, respectively. The factor C is a correction factor accounting for the effect of the wall on the drag as a function of $\tilde{W} = W/D$, which is given by

$$C = \left(\ln \tilde{W} - 0.9157 + 1.7244\tilde{W}^{-2} - 1.7302\tilde{W}^{-4} + 2.4056\tilde{W}^{-6} - 4.5913\tilde{W}^{-8} \right)^{-1}. \quad (30)$$

After some time, the particle reaches a terminal velocity due to the balance of gravitational and buoyancy forces and the drag force can be expressed as

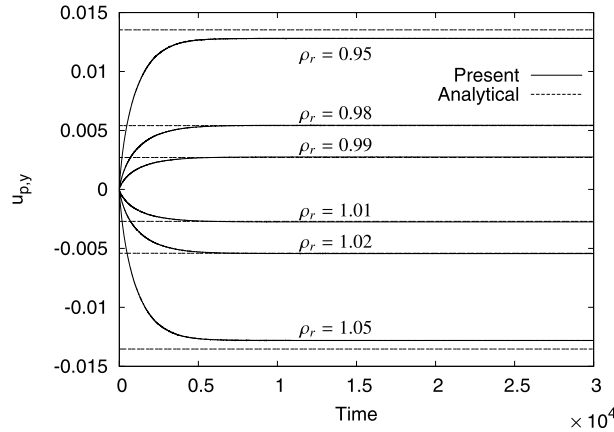


Fig. 9. Time evolution of the vertical velocity of a circular particle settling under gravity for different density ratios $\rho_r = \rho_p / \rho_f$.

$$\mathbf{F}_d = \frac{1}{4} \pi D^2 (\rho_f - \rho_p) \mathbf{g}. \quad (31)$$

Equating both expressions for the drag force yields the terminal sedimentation velocity

$$\mathbf{u}_t = \frac{D^2}{16C\nu} (1 - \rho_r) \mathbf{g}, \quad (32)$$

where $\rho_r = \rho_p / \rho_f$ is the ratio of the particle and fluid density. This approximate analytical solution serves as validation of the simulations.

The simulation parameters are identically chosen to those in the article of Wang et al. [40], where the kinematic viscosity is $\nu = 0.1$, the gravitational acceleration $g = 0.98 \cdot 10^{-4}$ and the non-dimensional channel width $\tilde{W} = 5$. In our simulations, the particle was resolved by a diameter of $D = 20$. The channel length is chosen sufficiently long for the particle to reach its terminal velocity and to minimize the influence of the inlet and the outlet condition. At all times, the particle is at least $15D$ away from either the inlet or the outlet, which is believed to be sufficient to mimic an infinite channel. Various simulations for different density ratios and particle Reynolds numbers $Re_p = \|\mathbf{u}_t\| D / \nu$, corresponding to an ascending and a descending particle, were performed. In Fig. 9, the time evolution of the vertical particle velocity is depicted and compared to its analytical solution of the terminal sedimentation velocity as in Eq. (32). The results match well with the analytical solution. However, for larger values of $|1 - \rho_r|$, a deviation of the result to the analytical solution can be observed. A similar behavior was found by Wang et al. [40] and it was pointed out that for large $|1 - \rho_r|$, the particle Reynolds number becomes too large for the analytical solution as in Eq. (32) to be valid.

3.4. Flapping wing

The last test problem considered in this paper is the simulation of a flapping, elliptical wing in a stagnant fluid. This is not just a benchmark simulation but may be viewed as a first step towards the simulation of bio-inspired locomotion as the problem aims to mimic the wing motion of a hovering insect. The aerodynamic coefficients such as drag and lift are compared to similar studies by Eldredge [43], Wang et al. [44] and Wu et al. [45], where a vortex particle method, a finite-difference scheme and a variant of the immersed-boundary lattice Boltzmann method were employed, respectively. Additionally, in the article of Wang et al. [44], the results of the two-dimensional simulations were compared to the corresponding three-dimensional experiment.

The elliptical wing has an aspect ratio of 10 and follows a sinusoidal translational and rotational pitching motion. With the center position $(x(t), y(t))$ and the wing orientation $\alpha(t)$ with respect to the x -axis, the motion may be modeled as

$$x(t) = \frac{A_0}{2} \cos(2\pi f t), \quad y(t) = \text{const}, \quad (33)$$

$$\alpha(t) = \alpha_0 + \beta \sin(2\pi f t + \phi), \quad (34)$$

where A_0 , f , α_0 , β and ϕ denote the maximum stroke amplitude, the frequency, the initial angle of attack, the pitching amplitude and the phase difference between rotation and translation, respectively. The Reynolds number is defined by means of the maximum translational velocity of the wing and the chord c as $Re = u_{\max} c / \nu = \pi f A_0 c / \nu$. For comparison, all parameters in our simulations are equivalent to those used by Eldredge [43], Wang et al. [44] and Wu et al. [45]. This yields a Reynolds number of $Re = 75$, a maximum amplitude $A_0 = 2.8c$ and the parameters α_0 , β are chosen to be $\pi/2$ and $\pi/4$, respectively. In the present simulations, a maximum velocity of $u_{\max} = 0.01$, a chord length of $c = 40$ and a square domain of size $H \times W = 25c \times 25c$ have proven to be sufficient. The phase difference ϕ is known to be a crucial

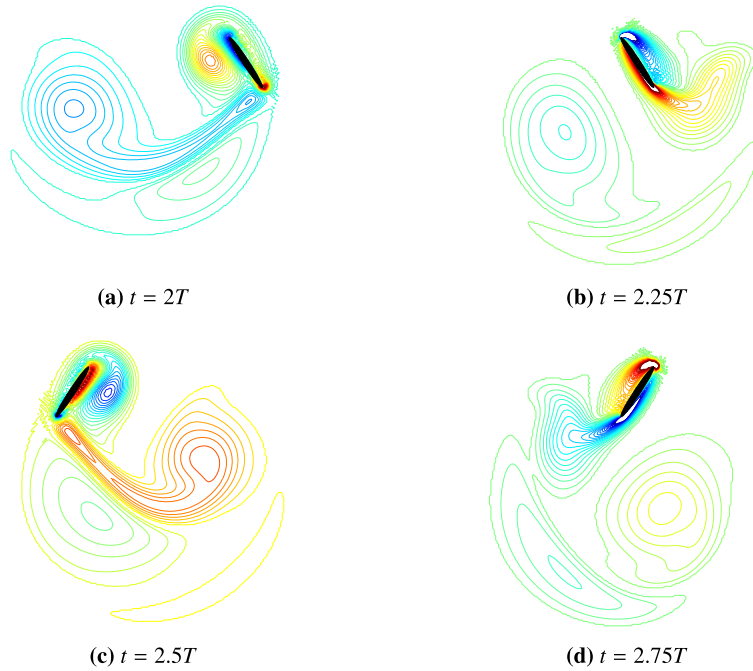


Fig. 10. Vorticity contour plots for the advanced rotation with $\phi = \pi/4$. The colors red and blue correspond to positive and negative vorticity, respectively.

parameter as it changes the characteristics of the aerodynamic forces significantly. Hence, we investigate an advanced and a delayed rotation with respect to the translational motion corresponding to $\phi = \pi/4$ and $\phi = -\pi/4$, respectively. As an example, the vorticity contours for the third cycle and a phase difference of $\phi = \pi/4$ are shown in Fig. 10. In the beginning of each new cycle, two dominant vortex structures can be observed, where one with a positive circulation is attached to the lower edge of the wing and the other one corresponds to the starting vortex with a negative circulation (see Fig. 10a). In the subsequent acceleration in negative x-direction, the vortex with positive circulation is absorbed into the boundary layer and a new vortex with negative vorticity is formed on the leading edge. Meanwhile, the starting vortex is shed from the trailing edge and begins to propagate downwards (see Fig. 10b). The pattern is then repeated for the second half of the cycle. For subsequent strokes, the vortex structures shed from the wing continue to travel downwards but dissipate quickly due to the low Reynolds number and no noteworthy increase of the wake in the far field is observed. It is noted that analogous phenomena were found in the work of Eldredge [43], to which we refer for a more detailed physical interpretation. For a phase difference of $\phi = -\pi/4$, the vorticity contours are depicted in Fig. 12. The mechanisms of vortex formation and absorption are equivalent. However, due to the large angle of attack at the end of each stroke, the vortices separate much earlier than in the case of an advanced rotation. This is clearly visible for the vortex attached to the leading edges with negative circulation as shown in Fig. 12b. After formation due to the translational acceleration, this vortex almost immediately separates from the leading edge of the wing (see Fig. 12c). As a result, more compact coherent vortex structures with stronger circulation are formed. A periodic pattern is reached for both cases after a short time of approximately two cycles.

For a more quantitative comparison, Figs. 11 and 13 show the time series of the drag and the lift coefficient for the advanced and the delayed rotation, respectively. As suggested by Wang et al. [44], the aerodynamic forces are normalized by the maxima of the corresponding quasi-steady forces in order to scale out the geometrical properties of the wing. For this purpose, the quasi-stationary, non-dimensional coefficients are approximated by $C_L = 1.2 \sin(2\alpha)$ and $C_D = 1.4 - \cos(2\alpha)$. The comparison of Fig. 11 and Fig. 13 highlights the significant influence of the phase difference between translation and rotation on the aerodynamic forces, as the corresponding time series of lift and drag coefficients have a fundamentally different characteristics. Furthermore, the averaged values exhibit a similar behavior, where $(\bar{C}_{D,a} = 0.603, \bar{C}_{L,a} = 0.540)$ and $(\bar{C}_{D,d} = 0.602, \bar{C}_{L,d} = 0.063)$ were found for the advanced and the delayed rotation, respectively. Most noteworthy is the sensitivity of the average lift coefficient to the kinematics, which is significantly smaller for a delayed rotation of the wing. This is intuitive, since the wing motion in both cases mainly differ by the angle of attack at the end of the stroke, namely $\pi/4$ and $3\pi/4$ for $\phi = \pi/4$ and $\phi = -\pi/4$, respectively. As a result, this yields a negative lift and a much earlier flow separation in the case of a delayed rotation as the angle of attack is larger than $\pi/2$. As it is illustrated in Fig. 11, the drag and lift histories for the case of the $\phi = \pi/4$ are in good agreement with both reference cases. The time series follow the results of Eldredge [43] especially close. Similarly, a reasonable match is achieved for the delayed rotation as shown in Fig. 13. The most substantial discrepancy is observed for the lift force. A difference for both references in phase and magnitude is noticeable. However, our results have the same phase as those of Wu et al. [45] and the difference in amplitude is comparable to the difference between the two references.

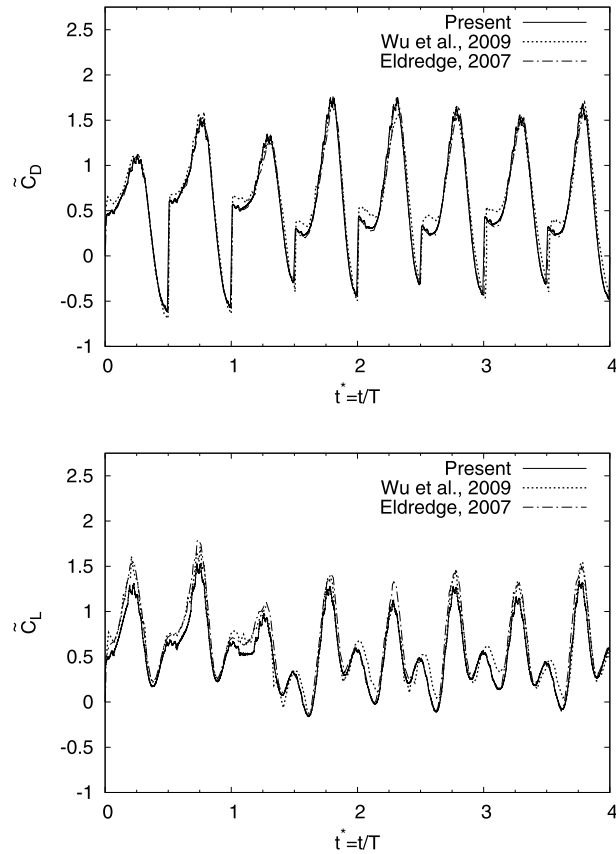


Fig. 11. Evolution of the drag and lift coefficient for a phase difference of $\phi = \pi/4$.

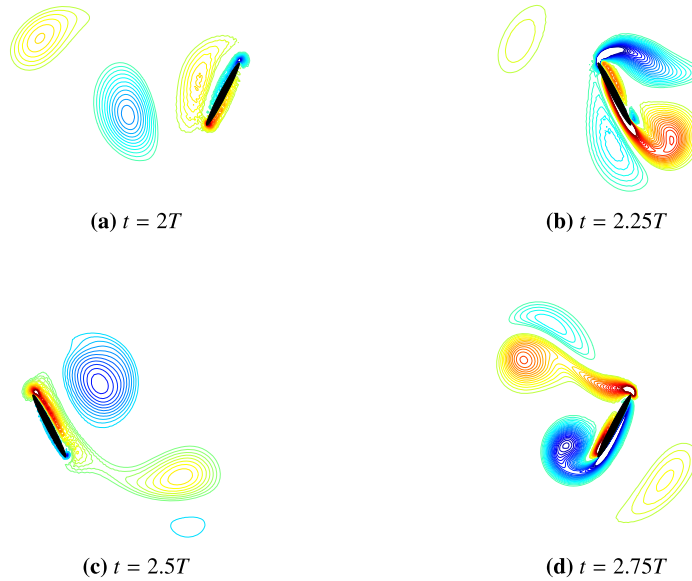


Fig. 12. Vorticity contour plots for the delayed rotation with $\phi = -\pi/4$. The colors red and blue correspond to positive and negative vorticity, respectively.

4. Concluding remarks

In this work, we have presented an accurate and robust numerical scheme for the treatment of complex, non-stationary wall boundaries, which is compatible with the entropic lattice Boltzmann method. The Grad's ten moment approximation

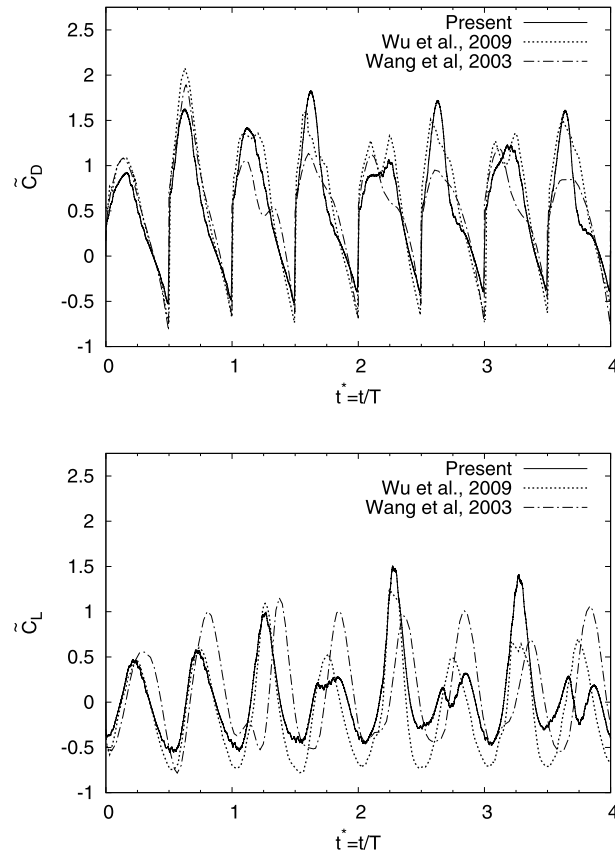


Fig. 13. Evolution of the drag and lift coefficient for a phase difference of $\phi = -\pi/4$.

which was earlier used to represent missing populations at open outlets provide a good estimate for the missing populations at the wall boundary nodes also. Furthermore, an extension to treat moving boundaries is proposed, by taking the momentum exchange between the boundary and the fluid as well as the local density alteration due to the displacement of mass into account. In summary, we obtained a second order accurate scheme, which resolves stability issues of existing Cartesian grid approaches such as IBB (see Sections 3.1 and 3.2).

For validation, various simulations were performed and compared to data found in the literature. First, the standard benchmark of a flow past a stationary, circular cylinder was performed in order to assess the accuracy and stability without the additional complication of a moving boundary. Since a good agreement to the literature was found, simulations of moving objects such as a transversely oscillating cylinder, a sedimenting circular particle and a flapping wing were considered. In all cases, the results compared well with the existing literature.

Although we have found consistent results for all simulations, there are still aspects which need to be considered in future work. For instance, the most significant advantage of ELBM is the ability to simulate turbulence at high Reynolds numbers without additional sub-grid models. As turbulence is inherently three-dimensional, the accuracy and the stability of the proposed scheme need to be confirmed in a three-dimensional setup with high Reynolds numbers in combination with the ELBM. The extension to three-dimensional space is straightforward as the proposed scheme is independent of the lattice and the dimensionality of the system. A three-dimensional version is already implemented and being tested; the result will be published in a subsequent paper. Furthermore this boundary condition shall be tested on other entropy based models such as the Karlin–Bösch–Chikatamarla (KBC) model [46] and other multispeed lattices [47]. This will be the focus of our future efforts.

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