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DISCRETE ARTIFICIAL BOUNDARY CONDITIONS FOR THE LATTICE BOLTZMANN METHOD IN 2D

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Abstract. To confine a spatial domain to a smaller computational domain, one needs artificial boundaries. This work considers the lattice Boltzmann method and deals with boundary conditions for these open boundaries. Ideally, such a condition does not interact with the fluid at all. We present a novel two-dimensional discrete artificial boundary conditions to pursue that goal and we discuss four different versions. This type of condition is formulated on the discrete lattice Boltzmann level and does not require a PDE formulation of the fluid. We set a special focus on the D2Q9 model. Our numerical results compare the novel discrete artificial boundary conditions to simulations using the existing non-reflecting characteristic boundary condition.

1. INTRODUCTION

In the field of computational fluid dynamics, the lattice Boltzmann (LB) method is a widely used and a flexible tool. Not only its ease of implementation, but also its applicability to complex flows make the LB method attractive for real-world simulations. Applications are found in acoustics (e.g., [1]), blood flow (e.g., [2]) and fluid-structure interaction (e.g. [3]) (among many others).

To achieve an efficient numerical simulation, often the fluid domain is confined to a smaller computational domain. Thereby, some non-physical boundaries, so-called artificial boundaries, occur. Using standard boundary conditions (e.g., a pressure or velocity condition) at open boundaries, the boundaries behave in an unphysical manner: spurious waves are reflected. An ideal boundary condition at artificial boundaries does not create any spurious effects, which influence the simulation results. For the LB method often boundary conditions are derived from known macroscopic physical conditions. However, the problem of finding correct artificial boundary conditions (ABCs) holds also on the macroscopic scale, not only on the mesoscopic scale of the LB method.

Several studies have been made for artificial boundaries. A review on absorbing boundary conditions for hyperbolic systems can be found in [4]. Hedstrom [5] and Thompson [6] developed *characteristic boundary conditions* (CBCs) for hyperbolic equations. In the LB method, one has to transfer any macroscopic formulation of an ABC to the mesoscopic level. Non-reflecting CBCs were

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adapted for the LB method [7–9] and create much smaller spurious effects than standard boundary conditions. To avoid a macroscopic formulation, we presented the first one-dimensional ABCs on the discretized LB formulation in earlier works [9,10]. In the current work these discrete artificial boundary conditions (DABCs) are transferred and applied to two-dimensional LB simulations.

This article is structured as follows. In Section 2 we briefly explain the LB method, focusing on the D2Q9 model. The two-dimensional DABCs are constructed in Section 3. This paper ends with the presentation of numerical test results (Section 4) and with conclusions (Section 5).

2. The Lattice Boltzmann Method

We briefly summarize the lattice Boltzmann (LB) method in the two-dimensional space. Based on the chosen discretization one has q discrete velocities $\vec{c_i}$, $i = 0, \ldots, q-1$ in the LB method. This yields the D2Qq LB model (notation proposed by Qian et al. [11]). As one specific example, the popular D2Q9 model is given by the discrete velocities

$$\vec{c}_0 = \vec{0}, \qquad \vec{c}_i = c \begin{pmatrix} \cos\left(\frac{\pi}{2}(i-1)\right) \\ \sin\left(\frac{\pi}{2}(i-1)\right) \end{pmatrix}, \qquad \vec{c}_j = \sqrt{2}c \begin{pmatrix} \cos\left(\frac{\pi}{2}(j-\frac{1}{2})\right) \\ \sin\left(\frac{\pi}{2}(j-\frac{1}{2})\right) \end{pmatrix}, \qquad (1)$$

with i = 1, 2, 3, 4 and j = 5, 6, 7, 8. Here, the parameter $c \neq 0$ scales the velocities. Given a regular lattice, the space points are denoted by \vec{x}_n and time points by t_s . The set of all considered space points is denoted by $\mathcal{G}_x = \{\vec{x}_n\}$. In the LB method, the temporal evolution of so-called *populations* $f_i = f_i(\vec{x}_n, t_s)$ is computed for each lattice node \vec{x}_n and time t_s . That is, $f_i(\vec{x}_n, t_s)$ gives the number density (scaled by mass) of fictitious particles with velocity \vec{c}_i at each lattice node (\vec{x}_n, t_s) . The evolution of populations is described by the LB equation, which defines an update rule of the populations based on particles' collision and streaming (see also, e.g., [12–14] for more details):

$$f_i(\vec{x}_n + \vec{c}_i, t_{s+1}) = f_i(\vec{x}_n, t_s) + C_i(f(\vec{x}_n, t_s)), \quad \text{for} \quad i = 0, \dots, q-1.$$
(2)

Here the vector $\vec{f}(\vec{x}_n, t_s)$ gathers all populations at the lattice node (\vec{x}_n, t_s) . It is required that the lattice nodes \vec{x}_m fulfill the condition

$$\vec{x}_m = \vec{x}_n + \vec{c}_i, \quad \text{for } i \in \{0, \dots, q-1\},$$
(3)

such that particles move in one time step $t_s \to t_{s+1}$ exactly from one node to an adjacent node. The right hand side of (2) gives the populations after particle collisions, hence C_i models the change due to collision. A very popular choice for C_i is given by the BGK scheme [15], which is a single relaxation time (SRT-BGK) model. There are also models with more relaxation parameters, e.g., the multiple relaxation time model [16] and the two-relaxation time model [17].

Using the SRT-BGK model, the LB equation (2) reads

$$f_i(\vec{x}_n + \vec{c}_i, t_{s+1}) = (1 - \omega)f_i(\vec{x}_n, t_s) + \omega f_i^{\text{eq}}(\vec{x}_n, t_s),$$

where $f_i^{\text{eq}}(\vec{x}_n, t_s)$ is a local equilibrium distribution and $\omega = 1/\tau$ a free relaxation parameter. For example in the D2Q9 model, the equilibrium reads

$$f_i^{\rm eq}(\vec{x}_n, t_s) = E_i(\rho, \vec{u}) := w_i \rho \left[1 + 3\frac{\vec{c}_i \cdot \vec{u}}{c^2} + \frac{9}{2c^4}(\vec{c}_i \cdot \vec{u})^2 - \frac{3}{2}\frac{|\vec{u}|^2}{c^2} \right]$$
(4)

with weights $w_0 = \frac{4}{9}$, $w_{1-4} = \frac{1}{9}$ and $w_{5-8} = \frac{1}{36}$ and fluid quantities

$$\rho(\vec{x}_n, t_s) = \sum_{i=0}^{q-1} f_i(\vec{x}_n, t_s), \qquad \vec{u}(\vec{x}_n, t_s) = \begin{pmatrix} v(\vec{x}_n, t_s) \\ w(\vec{x}_n, t_s) \end{pmatrix} = \frac{1}{\rho(\vec{x}_n, t_s)} \sum_{i=1}^{q-1} \vec{c}_i f_i(\vec{x}_n, t_s). \tag{5}$$

The fluid quantities are then approximations to the solution of the Navier-Stokes equations. This can be verified with help of a Chapman-Enskog expansion or other asymptotic analyses [18, 19]. Note that the arguments (\vec{x}_n, t_s) were suppressed in (4) for better readability.

The LB method requires the presence of all q populations in all grid points at any time. This requirement is ensured by the LB equation, provided condition (3) holds. Condition (3) is satisfied at least for all interior nodes, but is not for those near the boundary of the computational domain. In fact, we define a boundary node by the lack of some adjacent nodes. That is, a node $\vec{x}_b \in \mathcal{G}_x$ of the spatial discretization is said to be a boundary node if $\vec{x}_b + \vec{c}_i \notin \mathcal{G}_x$ for at least one discrete velocity \vec{c}_i . If \vec{c}_k is such a velocity (i.e., $\vec{x}_b + \vec{c}_k \notin \mathcal{G}_x$), then a boundary condition for $f_{\vec{k}}(\vec{x}_b, \cdot)$ is needed, where \vec{k} denotes the index defined by $\vec{c}_{\vec{k}} = -\vec{c}_k$. These unknown populations can be computed, e.g., by specifying a fluid pressure or velocity [20,21]. The desired condition depends on the kind of the boundary. If the boundary is given physically as a wall, then often no-slip boundary conditions are applied. For open boundaries, which are not aligned with a physical boundary, sometimes periodic boundary conditions are reasonable. Applying a pressure or a velocity condition at these lattice sites will generate undesired, spurious reflections. In the following, we present a further approach, which aims at computing the unknown populations for open boundaries such that preferably no reflection in the fluid quantities (5) occurs. In this sense, such a boundary represents the physically correct behavior.

3. DISCRETE ARTIFICIAL BOUNDARY CONDITION

Next, we determine the unknown populations of boundary nodes in a two-dimensional LB simulation for an open boundary by generalizing our one-dimensional approach [10].

3.1. Basic approach of Discrete Artificial Boundary Conditions

Let $\Gamma = \{\vec{x}_k \in \mathcal{G}_x \mid \vec{x}_k \text{ is a boundary node}\}\$ be the set of all boundary nodes. Then at all $\vec{x}_b \in \Gamma$ there are some populations which have to be computed by a boundary condition. However, for the moment we restrict our explanation to those boundary nodes $\Gamma_{\rm E} \subset \Gamma$ of a rectangular domain, for which a right adjacent node is missing, i.e., $\vec{x}_b^{\rm E} \in \Gamma_{\rm E}$ if and only if $\vec{x}_b^{\rm E} + \vec{c}_k \notin \mathcal{G}_x$ and $\vec{c}_k \cdot (1, 0)^{\rm T} > 0$. The situation is sketched in Fig. 1, where periodic boundary conditions are assumed to hold at the top and bottom of the computational domain. This assumptions avoids having corners, which will be considered later. For the D2Q9 model (1), the task of the boundary condition in these nodes is to assign the populations $f_{3,6,7}(\vec{x}_b^{\rm E}, t_s), \vec{x}_b^{\rm E} \in \Gamma_{\rm E}$ (for any time level $t = t_s$). We return to a general formulation afterwards.

A novel discrete boundary condition for one-dimensional LB simulations was developed by the authors in [10]. There, the unknown populations at boundary nodes are derived by considering LB subproblems. We follow the same idea to construct a boundary condition in two space dimensions. This means we solve two-dimensional LB subproblems to obtain the unknown populations. For all time levels, individual subproblems are considered separately. Therefore all subproblems are labeled: the s-th subproblem is used to compute all unknown populations at time $t = t_s$.

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FIGURE 1. Beyond the boundary of the computational domain are fictitious nodes (\Box) . They are used in the computation of the subproblems.

We explain the procedure in detail for $\Gamma_{\rm E}$ and the D2Q9 case. The s-th subproblem consists of H(s) fictitious layers of nodes in x_1 -direction, where H(s) is arbitrary (and may vary with time t_s), see Fig. 1. We suggest to allow a maximal size $H_{\rm max}$ during the whole simulation and use $H(s) = \min\{s, H_{\rm max}\}$. The uncapped choice H(s) = s (for all $s \in \mathbb{N}$) would result in an ideal boundary condition, however the computational effort would be too high.

Now, let the set of fictitious nodes be denoted by \mathcal{F}_x^s . Then the subproblem's domain \mathcal{G}_x^s is given by interface nodes $\Gamma_{\rm E}$ and the fictitious lattice extension: $\mathcal{G}_x^s = \Gamma_{\rm E} \cup \mathcal{F}_x^s$. In Fig. 1 these nodes are inside the dashed rectangle. In the *s*-th LB subproblem the populations shall be denoted by $h_i^s(\vec{x}_m, t_k), \ \vec{x}_m \in \mathcal{G}_x^s$. Their evolution is also described by (2) (with f_i replaced by h_i^s). The LB equation is applied H(s) times. By this rule we proceed H(s) time levels starting from the subproblem's initial time $t_0^s := t_{s-H(s)}$. I.e., the time points for the *s*-th subproblem are $t_k \in$ $\{t_{s-H(s)}, \ldots, t_s\}$. After H(s) applications of (2), we achieve the unknown populations by

$$f_{3,6,7}(\vec{x}_b^{\rm E}, t_s) = h_{3,6,7}^s(\vec{x}_b^{\rm E}, t_s), \quad \vec{x}_b^{\rm E} \in \Gamma_{\rm E}.$$
(6)

This equation already formulates the discrete artificial boundary condition (DABC).

3.2. Well-definedness

The subproblems are well defined when there is an initialization rule for all populations and when boundary conditions for some h_i^s are formulated. The initialization is the crucial part of the DABC, since all errors are caused here. There is no general approach for finding appropriate populations for the initialization of the subproblem. An ideal initialization strongly depends on the processes in the computational domain. If no better information is available, we propose two strategies for the initialization of the subproblems:

$$h_i^s(\vec{x}_m, t_0^s) = E_i(\rho^s, \vec{u}^s), \quad \forall \vec{x}_m \in \mathcal{F}_x^s, \tag{7}$$

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with ρ^s and \vec{u}^s to be chosen appropriately or

$$h_i^s(\vec{x}_m, t_0^s) = f_i(\vec{x}_b^{\rm E}, t_0), \quad \forall \vec{x}_m \in \mathcal{F}_x^s, \quad \vec{x}_b^{\rm E} \in \Gamma_{\rm E} \text{ with } x_{m,\beta} = x_{b,\beta}^E, \tag{8}$$

where Greek indices denote the spatial coordinates. That is, a homogeneous equilibrium in (7) and a constant extrapolation orthogonal to the boundary in (8). Also other initializations are conceivable, e.g., a convex combination of the above both possibilities. Additionally, we always assign the populations at the interface nodes $\vec{x}_b^{\rm E} \in \Gamma_{\rm E}$ as follows (for all involved time levels)

$$h_i^s(\vec{x}_b^{\rm E}, t_k) = f_i(\vec{x}_b^{\rm E}, t_k), \quad i = 0, \dots, q-1, \quad t_k \in \{t_{s-H(s)}, \dots, t_{s-1}\}.$$
(9)

For the top and bottom boundary of the subproblem, we use here periodic boundary conditions, for simplicity. No boundary condition is required for the boundary nodes on the opposite site of $\Gamma_{\rm E}$ (that is the right boundary of the subproblem). This is, because from this boundary only information from time $t = t_0^s$ is affecting (6).

From (9) we see that the DABC takes past information up to H(s) time levels ago. For this reason the quantity H(s) is called the *history depth of the s-th subproblem* and H_{max} is denoted as the maximal history depth.

3.3. Generalization

So far, the basic approach was explained for the right boundary of a rectangular computational domain with periodic boundaries at the top and bottom. In the following we generalize the approach of the DABC without any restrictions. There is a set of boundary nodes Γ , where the DABC should be used to compute the inward populations $f_k(\vec{x}_b, t_s)$ at time $t = t_s$. To this end, we consider a subproblem (the *s*-th subproblem), whose lattice consists of joint interface nodes $x_b \in \Gamma$ (\bullet in the figures) plus a set of fictitious nodes \mathcal{F}_x^s . The amount and location of the fictitious nodes depends on the problem and the chosen history depth H(s). We go into further detail in the subsequent subsection. The fictitious nodes have to be chosen such that after H(s) applications of the LB equation all required quantities are given.

Let us consider the application of the DABC for two adjacent boundaries as depicted in Fig. 2 (for the top and right boundary). This small example demonstrates that the treatment of corners requires to consider one subproblem to achieve all unknown populations. It is not possible to consider two independent subproblems, one for the top and right boundary each. After 5 streaming steps the information from the filled square node enters a boundary node on the right side. Hence, it is important that the fictitious nodes which extend the computational domain vertically and horizontally build a connected set of LB nodes.

Given the s-th subproblem, we perform H(s) iterations of it. For the interface nodes $x_b \in \Gamma$, we set all populations according to

$$h_i^s(\vec{x}_b, t_k) = f_i(\vec{x}_b, t_k), \quad i = 0, \dots, q - 1, \quad t_k \in \{t_{s-H(s)}, \dots, t_{s-1}\}.$$
(10)

At time $t_0^s = t_{s-H(s)}$ we also need an initialization for the subproblem's interior nodes, which is done, e.g., by adapting (7) or (8). After all H(s) iterations are done, the unknown populations of the original problem are obtained:

$$f_k(\vec{x}_b, t_s) = h_k^s(\vec{x}_b, t_s), \quad \vec{x}_b \in \Gamma.$$

$$\tag{11}$$

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FIGURE 2. Application of the DABC (H = 5) for two adjacent boundaries. Populations from the filled square node are tracked during the iteration of the subproblem.

3.4. Discrete Artificial Boundary Condition for a channel

With the basic approach of the DABC the existence of additional lattice nodes in the exterior of the actual computational domain is emulated. For each subproblem the amount of fictitious lattice nodes is chosen such that no other boundary of the subproblem affects the interface nodes (which is the boundary of the computational domain).

Let us consider a channel flow with the aim to apply the DABC at the right boundary of the channel. This means, the inward populations at \bigcirc -nodes have to be computed, see Figs. 3 and 4. In Fig. 3 the situation is sketched for a theoretical choice of fictitious nodes, having more nodes in x_2 -direction than the actual computational domain. Contrary, in Fig. 4 the fictitious nodes have equal number in x_2 -direction, but also channel walls are incorporated in the subproblem's domain (\blacktriangle and $\textcircled{\square}$ -nodes). Both cases represent a well defined situation (cf. Section 3.2), however only Fig. 4 seems to be physically reasonable.

This example demonstrates that there is no general rule for the subproblems. It is recommend to choose the subproblems the same way as a logical enlargement of the computational domain would be. The situation of Fig. 3 represents an outlet of a channel, whereas in Fig. 4 the boundary of the computational domain is within the channel.

3.5. Computational costs

The specific computational effort of the DABC depends on the LB model in use. Therefore we do not count arithmetic operations here. At each time level a LB subproblem is solved. It is possible to align the collision and streaming steps with those of the original problem. A detailed description of this procedure is given in [10]. This means the DABC can be parallelized in the same way as the main LB simulation. In this implementation strategy, one has to treat at most H_{max} subproblems

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FIGURE 3. Application of DABC (here H = 4) at the right boundary of a channel. There are no channel walls in the subproblem.

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FIGURE 4. Application of DABC (here H = 4) at the right boundary of a channel. In the subproblem's domain there are also channel walls.

simultaneously. If each subproblem consists of $J := \# \mathcal{G}_x^{\cdot}$ nodes, the total costs of the DABC are equivalent to a lattice enlargement by $H_{\max} \cdot J$ nodes.

4. Numerical results

Here we describe the working principle of the DABC by a visual interpretation and present results for two test scenarios for the D2Q9 model. To rate the performance and the errors of the (DABC), we compare our DABC results with results obtained from a constant pressure condition [20] and with results from a non-reflecting characteristic boundary condition (CBC) [9]. In fact, for the CBC at the right boundary of a rectangular computational domain, we numerically solve the system

$$\frac{\partial \vec{U}}{\partial t} + \begin{pmatrix} w & 0 & \rho \\ 0 & w & 0 \\ \frac{c_s^2}{\rho} & 0 & w \end{pmatrix} \frac{\partial \vec{U}}{\partial y} = - \begin{pmatrix} \frac{1}{2c_s^2} & 0 & \frac{1}{2c_s^2} \\ -\frac{1}{2\rho c_s} & 0 & \frac{1}{2\rho c_s} \\ 0 & 1 & 0 \end{pmatrix} \vec{\mathcal{L}}_x$$

at the boundary and transfer the outcome into a Dirichlet condition for the populations. Here $\vec{U}^{\top} = (\rho, v, w)$ is the vector of the fluid quantities (5) and $\vec{\mathcal{L}}_x$ denotes the wave amplitude variations:

$$\vec{\mathcal{L}}_{x} = \begin{pmatrix} \mathcal{L}_{x,1} \\ \mathcal{L}_{x,2} \\ \mathcal{L}_{x,3} \end{pmatrix} = \begin{pmatrix} \tilde{\lambda}_{1} \vec{\ell}_{1}^{\top} \frac{\partial \vec{U}}{\partial x} \\ \tilde{\lambda}_{2} \vec{\ell}_{2}^{\top} \frac{\partial \vec{U}}{\partial x} \\ \tilde{\lambda}_{3} \vec{\ell}_{3}^{\top} \frac{\partial \vec{U}}{\partial x} \end{pmatrix}, \quad \text{with } \tilde{\lambda}_{i} = \begin{cases} \lambda_{i} & \text{outgoing} \\ 0 & \text{incoming,} \end{cases} \begin{pmatrix} \vec{\ell}_{1}, \vec{\ell}_{2}, \vec{\ell}_{3} \end{pmatrix} = \begin{pmatrix} c_{s}^{2} & 0 & c_{s}^{2} \\ -c_{s}\rho & 0 & c_{s}\rho \\ 0 & 1 & 0 \end{pmatrix}$$

and eigenvalues $\lambda_1 = v - c_s$, $\lambda_2 = v$, $\lambda_3 = v + c_s$. For more details and the treatment of other boundaries we refer to [9].

4.1. Concentric wave

For the first numerical test, the initialization of the fluid is done by a Gaussian pressure pulse:

$$p(x,y) = p_0 + (p_{\max} - p_0) \exp\left(\frac{-(x^2 + y^2)}{2\sigma^2}\right).$$

The pressure values are related to the density by

$$p(x,t) = c_s^2 \rho(x,t) = \frac{1}{3} \rho(x,t),$$

We set $\sigma = 0.1$ and the pressures according to $\rho_0 = 1$, $\rho_{\text{max}} = 1.15$. The fluid velocity is homogeneously set to $\vec{u}(\cdot, t_0) = \vec{u}_0$ at initial time.

The rectangular lattice is chosen with 201×1001 nodes, representing the spatial domain $[-1, 1] \times [-5, 5]$. We apply periodic boundary conditions for the top and bottom boundary. A LB reference solution on a sufficiently larger domain is computed, such that errors

$$e_z(\vec{x}_n, t_s) := z(\vec{x}_n, t_s) - z^{\text{ref}}(\vec{x}_n, t_s), \quad \vec{x}_n \in \mathcal{G}_x, \ s \in \mathbb{N},$$
(12)

can be computed for any available quantity z (e.g., $z \in \{\rho, \vec{u}, f_i\}$). With help of the reference populations an ideal boundary condition is applied at left boundary nodes \vec{x}_b^{W} :

$$f_j(\vec{x}_b^{\mathrm{W}}, t_s) = f_j^{\mathrm{ref}}(\vec{x}_b^{\mathrm{W}}, t_s), \quad j \in \{1, 5, 8\}, \ s \in \mathbb{N}.$$

On the right boundary we apply the DABC or any other condition to be tested.

4.1.1. Visual interpretation

In Fig. 5 the density profile is plotted for different time levels. The maximal history depth is selected as $H_{\text{max}} = 40$ and the relaxation parameter in the illustration is $\omega = 1$. To give a visual





FIGURE 5. Temporal evolution of the density. Snapshots correspond to $t \in \{t_0, t_{100}, t_{185}, t_{255}, t_{400}\}$. A reflecting wave can be observed traveling from the right boundary into the interior.

interpretation of how the DABC is working, we consider the situation at time $t = t_{185}$. In fact, we zoom in to the section, which is marked in the third snapshot of Fig. 5. Therefore, in Fig. 6 the mass density ρ of the computational domain is shown at $t = t_{185}$. Moreover, the mass density in the 185-th subproblem is shown. On the different plots of Fig. 6 we see the mass density profile of the subproblem changing during the iterations of the subproblem. The first plot shows it at initialization, which is done by (7) and (10) ($\rho^s = 1$, $\vec{u}^s = \vec{u}_0 = \vec{0}$). Only the last plot is relevant for the desired populations, which are given by (11). We see that after the final iteration of the subproblem both regions match together. Thus, the DABC constructs a suitable extension of the computational domain in fictitious nodes, which provides then all information for the unknown populations. This interpretation clarifies that the initialization of subproblems determines the accuracy of the DABC.

4.1.2. Simulation results

In addition to Fig. 5 the errors e_{ρ} , e_v and e_w , cf. (12), are depicted in Fig. 7 for time $t = t_{400}$. The error plots shown in the left column correspond to the subproblem initialized by (7), which is here equivalent to (8) due to the choice of ρ^s and \vec{u}^s . Errors in the right column correspond to a modified initialization of (8), where the time of evaluation is not fixed (t_0^s instead of t_0):

$$h_i^s(\vec{x}_m, t_0^s) = f_i(\vec{x}_b^{\mathrm{E}}, t_0^s), \quad \forall \vec{x}_m \in \mathcal{F}_x^s, \quad \vec{x}_b^{\mathrm{E}} \in \Gamma_{\mathrm{E}} \text{ with } x_{m,\beta} = x_{b,\beta}^E.$$
(13)

For each error e_z we can see different shapes of the surfaces. It should be noted that the peaks are not located at the same points. As a further remark we emphasize that an initialization according to (13) created instabilities in the one-dimensional case [10].

In the sequel we consider normalized errors

$$N_{z}(t_{s}) := \|e_{z}(\cdot, t_{s})\|_{\ell_{2}} = \sqrt{\sum_{\vec{x}_{n} \in \mathcal{G}_{x}} \left(z(\vec{x}_{n}, t_{s}) - z^{\text{ref}}(\vec{x}_{n}, t_{s})\right)^{2}},$$
(14)

where z again can be replaced by any available quantity.



FIGURE 6. Temporal evolution of the subproblem $(x_1 \in [201, 241])$, which was initialized by (7)/(8).

In the one-dimensional case the error could be decreased by taking a larger history depth, see [10]. First we investigate if a similar behavior can be detected also in two space dimensions. Therefore, we consider the above test case repeatedly with different maximal history depths in the range from 4 to 80 and compute the corresponding errors N_z . The parameters chosen for the simulation are $\omega = 1$ and $\vec{u}_0 = 0$. Results are presented in Tables 1–3, which also contain reference values. That

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FIGURE 7. The left column shows the errors e_{ρ} , e_{v} and e_{w} (cf. (12)) when using the DABC with (7)/(8). Similarly, the right column shows errors when initializing with (13).

	Error $N_{\rho}(t)$ at					
	$t = t_{175}$	$t = t_{250}$	$t = t_{325}$	$t = t_{400}$		
Zou/He pressure	0.472981	0.678311	0.722984	0.723998		
CBC	0.016336	0.066936	0.108164	0.135353		
DABC H=4, $(7)/(8)$ DABC H=4, (13)	$\begin{array}{c} 0.016035 \\ 0.030312 \end{array}$	$\begin{array}{c} 0.077023 \\ 0.059209 \end{array}$	$\begin{array}{c} 0.119626 \\ 0.091554 \end{array}$	$\begin{array}{c} 0.146777 \\ 0.116822 \end{array}$		
DABC H=10, (7)/(8) DABC H=10, (13)	$\begin{array}{c} 0.011039 \\ 0.020151 \end{array}$	$\begin{array}{c} 0.065418 \\ 0.060705 \end{array}$	$\begin{array}{c} 0.107186 \\ 0.097759 \end{array}$	$\begin{array}{c} 0.134847 \\ 0.124270 \end{array}$		
DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.007960 \\ 0.015407 \end{array}$	$\begin{array}{c} 0.061694 \\ 0.062910 \end{array}$	$\begin{array}{c} 0.104964 \\ 0.102058 \end{array}$	$\begin{array}{c} 0.133531 \\ 0.129025 \end{array}$		
DABC H=40, (7)/(8) DABC H=40, (13)	$\begin{array}{c} 0.001986 \\ 0.007918 \end{array}$	$\begin{array}{c} 0.055666 \\ 0.070754 \end{array}$	$\begin{array}{c} 0.104786 \\ 0.114453 \end{array}$	$\begin{array}{c} 0.136482 \\ 0.141661 \end{array}$		
DABC H=80, (7)/(8) DABC H=80, (13)	$0.000002 \\ 0.000033$	$\begin{array}{c} 0.027226 \\ 0.075978 \end{array}$	$0.085173 \\ 0.145701$	$0.121441 \\ 0.173462$		

TABLE 1. Error N_{ρ} for different boundary conditions and time levels.

	Error $N_v(t)$ at				
	$t = t_{175}$	$t = t_{250}$	$t = t_{325}$	$t = t_{400}$	
Zou/He pressure	0.277485	0.359907	0.358679	0.345152	
CBC	0.009046	0.036197	0.048954	0.053523	
DABC H=4, $(7)/(8)$ DABC H=4, (13)	$\begin{array}{c} 0.009193 \\ 0.018250 \end{array}$	$\begin{array}{c} 0.041705 \\ 0.033751 \end{array}$	$\begin{array}{c} 0.055181 \\ 0.042891 \end{array}$	$\begin{array}{c} 0.059633 \\ 0.047084 \end{array}$	
DABC H=10, (7)/(8) DABC H=10, (13)	$\begin{array}{c} 0.006549 \\ 0.012309 \end{array}$	$\begin{array}{c} 0.036287 \\ 0.034344 \end{array}$	$\begin{array}{c} 0.049870 \\ 0.045440 \end{array}$	$\begin{array}{c} 0.054805 \\ 0.049971 \end{array}$	
DABC H= $20, (7)/(8)$ DABC H= $20, (13)$	$\begin{array}{c} 0.004842 \\ 0.009487 \end{array}$	$\begin{array}{c} 0.034892 \\ 0.035349 \end{array}$	$\begin{array}{c} 0.049417 \\ 0.047364 \end{array}$	$\begin{array}{c} 0.054755 \\ 0.052022 \end{array}$	
DABC H=40, $(7)/(8)$ DABC H=40, (13)	$\begin{array}{c} 0.001232 \\ 0.004922 \end{array}$	$\begin{array}{c} 0.032889 \\ 0.039249 \end{array}$	$\begin{array}{c} 0.051021 \\ 0.052736 \end{array}$	$\begin{array}{c} 0.057585 \\ 0.057175 \end{array}$	
DABC H= $80, (7)/(8)$ DABC H= $80, (13)$	$\begin{array}{c} 0.000001 \\ 0.000021 \end{array}$	$\begin{array}{c} 0.016820 \\ 0.046725 \end{array}$	$\begin{array}{c} 0.046855 \\ 0.071642 \end{array}$	$\begin{array}{c} 0.056847 \\ 0.075620 \end{array}$	

TABLE 2. Error N_v for different boundary conditions and time levels.

is, the errors obtained when using a Zou/He pressure boundary condition ($\rho = 1$ and $u_{\parallel} = 0$) [20], as well as a CBC (LODI) from [14] as described at the beginning of the current section. All in

	Error $N_w(t)$ at				
	$t = t_{175}$	$t = t_{250}$	$t = t_{325}$	$t = t_{400}$	
Zou/He pressure	0.078614	0.183191	0.225385	0.242753	
CBC	0.032066	0.050150	0.063324	0.074517	
DABC H=4, $(7)/(8)$ DABC H=4, (13)	$\begin{array}{c} 0.014582 \\ 0.005688 \end{array}$	$\begin{array}{c} 0.036721 \\ 0.028873 \end{array}$	$\begin{array}{c} 0.056772 \\ 0.047478 \end{array}$	$\begin{array}{c} 0.072032 \\ 0.061502 \end{array}$	
DABC H=10, (7)/(8) DABC H=10, (13)	$\begin{array}{c} 0.007677 \\ 0.004140 \end{array}$	$\begin{array}{c} 0.029861 \\ 0.028261 \end{array}$	$\begin{array}{c} 0.050469 \\ 0.049035 \end{array}$	$\begin{array}{c} 0.066239 \\ 0.064021 \end{array}$	
DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.002870 \\ 0.003158 \end{array}$	$\begin{array}{c} 0.024961 \\ 0.027737 \end{array}$	$\begin{array}{c} 0.047393 \\ 0.049795 \end{array}$	$\begin{array}{c} 0.064187 \\ 0.065342 \end{array}$	
DABC H=40, $(7)/(8)$ DABC H=40, (13)	$\begin{array}{c} 0.000325 \\ 0.001496 \end{array}$	$\begin{array}{c} 0.018999 \\ 0.028169 \end{array}$	$\begin{array}{c} 0.044452 \\ 0.052968 \end{array}$	$\begin{array}{c} 0.063156 \\ 0.069439 \end{array}$	
DABC H=80, (7)/(8) DABC H=80, (13)	$\begin{array}{c} 0.000000\\ 0.000006\end{array}$	$\begin{array}{c} 0.005729 \\ 0.022848 \end{array}$	$\begin{array}{c} 0.032076 \\ 0.056737 \end{array}$	$\begin{array}{c} 0.052336 \\ 0.075456 \end{array}$	

TABLE 3. Error N_w for different boundary conditions including DABCs with different history depths. All errors are given at four time levels.

all, the smallest errors are obtained when using the novel DABC with an initialization due to (7) respectively (8).

We see that the CBC and the DABC behave equally in N_{ρ} and N_{v} , whereas for N_{w} the DABC is superior. However, unlike the one-dimensional case, a significant decreasing influence of a larger history depth is not visible. The test case is challenging, because the wave is interacting with the boundary all the time, which is different to the one-dimensional test cases in [10]. In our opinion, this difference causes the missing decreasing influence of the history depth.

For the presentation of the next results we do not change the parameters. But, we fix the maximal history depth by $H_{\text{max}} = 20$ and vary the relaxation time $\tau = \frac{1}{\omega}$ from 0.6 to 1.5. The errors are computed at time $t = t_{400}$ and presented in Table 4. Note that the viscosity ν is related to the relaxation time as

$$\nu = \frac{2\tau - \Delta t}{6}c^2.$$

Hence, the concentric wave is decaying faster for larger values of τ , resulting in smaller errors, since already the wave interacting with the boundary is smaller.

The final result presented for the current test case fixes all parameters as before except for the initial fluid velocity \vec{u}_0 . The velocity component tangential to the boundary $(u_{0,\beta})$ is zero, whereas the component perpendicular to the boundary $(u_{0,\alpha})$ is varied. As before, errors are computed at $t = t_{400}$. When considering the errors, shown in Table 5, we see that the DABC, initialized with respect to (13), has clearly smaller errors for positive velocities. However the errors are larger for negative velocities. With initialization according to (7)/(8) the DABC behaves similar to the CBC.

		37 ()	NT (()	
		$N_{ ho}(t_{400})$	$N_v(t_{400})$	$N_w(t_{400})$
	Zou/He pressure	0.974653	0.464104	0.324983
- 0.60	CBC	0.172067	0.065029	0.092413
$\tau = 0.00$	DABC H= $20, (7)/(8)$	0.183732	0.071039	0.086858
	DABC H= $20, (13)$	0.178314	0.067579	0.086631
$\tau = 0.80$	Zou/He pressure	0.822321	0.391664	0.275049
	CBC	0.150659	0.058254	0.082080
	DABC H= $20, (7)/(8)$	0.152543	0.060856	0.072713
	DABC H= $20, (13)$	0.148096	0.057966	0.073507
	Zou/He pressure	0.639278	0.305219	0.214941
- 1.05	CBC	0.121525	0.049330	0.067567
$\tau = 1.23$	DABC H= $20, (7)/(8)$	0.117714	0.049754	0.057141
	DABC H= $20, (13)$	0.112726	0.047065	0.058467
	Zou/He pressure	0.578431	0.276624	0.195010
150	CBC	0.111281	0.046274	0.062339
7 = 1.00	DABC H= $20, (7)/(8)$	0.106612	0.046287	0.052214
	DABC H= $20, (13)$	0.101099	0.043626	0.053633

TABLE 4. Errors N_{ρ} , N_{v} and N_{w} for different boundary conditions and relaxation times.



FIGURE 8. Simulation setting of the second test case. The snapshot shows the modulus of the velocity and displays a vortex.

4.2. Flow past an obstacle in channel

In the second test example we simulate a flow past a square obstacle in a channel at Re = 100. The square obstacle has a dimension of L = 15 lattice nodes. The width and total length of the channel are 5L and 11L, respectively. It is displaced vertically by $\frac{L}{5}$ lattice nodes from the center of the channel, to break symmetry and allow a vortex street to develop. We place the obstacle 3L nodes from the inlet (left boundary), such that there are 7L lattice nodes behind the obstacle in direction of the flow. See also Fig. 8 for a visualization of the setting. Normally in a simulation, the right boundary would have a larger distance to the obstacle, but in the scope of testing a boundary condition the choice seems reasonable. At the inlet we impose a parabolic velocity profile with its maximal velocity $u_{\text{max}} = \frac{1}{9}$ in the center, whereas the velocity component in y-direction is set to zero. [20]. For the right boundary of the computational domain we test several DABCs and

		$N_{\rho}(t_{400})$	$N_v(t_{400})$	$N_w(t_{400})$
$u_{0,\alpha} = -0.20$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.761080\\ 0.082773\\ 0.076132\\ 0.159738\end{array}$	$\begin{array}{c} 0.360090\\ 0.039248\\ 0.037925\\ 0.081832 \end{array}$	$\begin{array}{c} 0.294364 \\ 0.079130 \\ 0.067832 \\ 0.086171 \end{array}$
$u_{0,\alpha} = -0.10$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.729659 \\ 0.107232 \\ 0.102220 \\ 0.150410 \end{array}$	$\begin{array}{c} 0.341081 \\ 0.044476 \\ 0.044317 \\ 0.063511 \end{array}$	$\begin{array}{c} 0.259046 \\ 0.071911 \\ 0.060727 \\ 0.081461 \end{array}$
$u_{0,\alpha} = -0.05$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.695514 \\ 0.116508 \\ 0.112323 \\ 0.134400 \end{array}$	$\begin{array}{c} 0.328143 \\ 0.046956 \\ 0.047139 \\ 0.055193 \end{array}$	$\begin{array}{c} 0.239728 \\ 0.068698 \\ 0.057872 \\ 0.071381 \end{array}$
$u_{0,\alpha} = 0.05$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.606929\\ 0.120947\\ 0.126173\\ 0.096058\end{array}$	$\begin{array}{c} 0.293510\\ 0.051021\\ 0.054359\\ 0.041342 \end{array}$	$\begin{array}{c} 0.198921 \\ 0.062830 \\ 0.059037 \\ 0.047969 \end{array}$
$u_{0,\alpha} = 0.10$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.556697 \\ 0.125892 \\ 0.129904 \\ 0.077947 \end{array}$	$\begin{array}{c} 0.273143 \\ 0.055574 \\ 0.058062 \\ 0.035392 \end{array}$	$\begin{array}{c} 0.177444 \\ 0.059419 \\ 0.057923 \\ 0.037626 \end{array}$
$u_{0,\alpha} = 0.20$	Zou/He pressure CBC DABC H=20, $(7)/(8)$ DABC H=20, (13)	$\begin{array}{c} 0.453472 \\ 0.136904 \\ 0.133179 \\ 0.049582 \end{array}$	$\begin{array}{c} 0.230098 \\ 0.065509 \\ 0.064572 \\ 0.025437 \end{array}$	$\begin{array}{c} 0.134056 \\ 0.054637 \\ 0.051532 \\ 0.022306 \end{array}$

TABLE 5. Errors N_{ρ} , N_{v} and N_{w} for different boundary conditions and fluid velocities u_{0} .

compare the errors (14) with those when using a CBC. We initialize the fluid in the interior of the computational domain with the same parabolic velocity profile and a decreasing density from inlet to outlet. The decay is chosen such that the resulting pressure gradient fits to the stationary solution of the Poiseuille flow when there would not be an obstacle [22].

We tested several versions of the DABC. They differ in the choice of the subproblem's initialization and the maximal history depth. In the following we refer to the different initialization strategies by DABC- $n, n \in \{1, 2, 3, 4\}$. Hereby, DABC-1 uses the strategy (7) with $\rho^s \equiv \rho(\vec{x}_b, t_0)$ and $\vec{u}^s = \vec{0}$. The second initialization type DABC-2 is given by (8), and DABC-3 is using the modification (13). Finally, DABC-4 can be written shortest in terms of the reference solution

$$h_i^s(\vec{x}_m, t_0^s) = f^{\text{ret}}(\vec{x}_m, t_0)$$



FIGURE 9. Normalized errors (14) $(N_{\rho}, N_v \text{ and } N_w)$ for DABCs two initialization strategies. Three different maximal history depths H_{max} were tested (10, 20 and 70). Also errors of a CBC are shown.

which, thereby, is very similar to DABC-2. The sole exception is that the density is decreasing in DABC-4, whereas it is has a constant level in DABC-2. Note, that the choice DABC-4 is not requiring a reference solution, it is only a logical extension of the interior initialization. Also note, that DABC-1 and DABC-2 coincided in the previous test case, but differ in the current test.

The plots in Fig. 9 show the errors (14) of DABC-2 using different maximal history depths. We clearly observe, that higher history depths result in smaller errors. They all are smaller than the reference error of a non-reflecting CBC. Although a difference between errors of DABC-2 and DABC-4 could not be detected visually, the errors of DABC-2 are a minimal smaller. The error plots of DABC-4 are not shown, since they look equally to DABC-2. As in the one-dimensional case, DABC-3 shows instabilities and thus corresponding error plots are omitted.

Already at the beginning of the simulation, using the DABC-1 there is a pressure wave generated at the right boundary traveling into the domain. By this, the whole density level is increased and remains on a higher niveau. This makes a consideration of N_{ρ} worthless. The pressure wave also affects the velocity profile for v, as one can see in the left plot of Fig. 10. As before, the same influence of the maximal history depth is also visible for DABC-1. The errors are significantly higher compared to DABC-2 and DABC-4.

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FIGURE 10. Normalized errors (14) (N_v and N_w) for DABC-1 and three maximal history depths H_{max} (10, 20 and 70). Plot also contain errors of a CBC.

All in all, in both test cases the initialization strategy (8) (DABC-2 in the second test case) produces good results.

5. Conclusions

In this work, the one-dimensional discrete artificial boundary condition (DABC) for the lattice Boltzmann (LB) method [10] was successfully transferred to two space dimensions. Our formulation of the DABC was done in a general way, but we set a special focus on the D2Q9 LB model. For the implementation of the DABC, the LB method was equipped with a so-called subproblem in each time step, which offers a free parameter, called the history depth. This tuning parameter determines the number of past time levels, which are taken into account in the subproblems. In addition, this parameter fixes the size of the subproblems, and thus it determines both, the accuracy and the computational effort of the DABC. Comparing the DABC with an ideal transparent boundary condition, any error is caused already in the initialization phase of these subproblems.

In the one-dimensional case, the history depth could be tuned to control the error. We presented two test cases, a two-dimensional Gaussian pressure pulse and a flow past an obstacle in a channel. The results of the second test case demonstrated that the history depth controls the error also for the two-dimensional DABC. By the first test, we could explain the working principle of the DABC: the solutions of the subproblems are shaped in such a way that they virtually extend the computed solution of the (actual) computational domain. Then, for the boundary of the computational domain, all missing information are taken from the subproblems.

The numerical tests showed that our proposed initialization strategy (8) leads to errors smaller than those obtained by characteristic boundary conditions.

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