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Momentum transfer correction for macroscopic-gradient boundary conditions in lattice Boltzmann methods

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The boundary conditions used to represent macroscopic-gradient-related effects in arbitrary geometries with the lattice Boltzmann methods need a trade-off between the complexity of the scheme, due to the loss of localness and the difficulties for directly applying link-based approaches, and the accuracy obtained. A generalization of the momentum transfer boundary condition is presented, in which the arbitrary location of the boundary is addressed with link-wise interpolation (used for Dirichlet conditions) and the macroscopic gradient is taken into account with a finite-difference scheme. This leads to a stable approach for arbitrary geometries that can be used to impose Neumann and Robin boundary conditions. The proposal is validated for stress boundary conditions at walls. Two-dimensional steady and unsteady configurations are used as test case: partial-slip flow between two infinite plates and the slip flow past a circular cylinder.

1. Introduction

Lattice Boltzmann (LB) methods [1–4] are an efficient approach to simulate fluid flow based on the solution of the Boltzmann equation with a minimal discretization of the velocity space [5]. One of its strengths is the ability to simulate complex geometries with little additional computational effort. Simulations with detailed geometries of porous media [6], blood vessels [7], indoor environments [8] or flow aerodynamics [9] are some successful examples. Different implementations of Dirichlet conditions for arbitrary geometries have been developed; however, little research has been published related to the implementation of Neumann boundary conditions. This deficit is probably due to several factors, which can be illustrated using the stress boundary-condition as an example. First, the stresses are macroscopic moments related to the non-equilibrium part of the distribution functions that have an $O(\partial_j u_i)$ influence on the accuracy of the boundary condition, which is sometimes neglected; additionally, many configurations do not require these kind of boundary conditions, and in the most common case where it is needed (i.e. zero tangential stresses for symmetry planes) the link-based approach can be applied through a specular reflection; furthermore, it is a hydrodynamic boundary condition, and kinetic ones are often preferred (especially for microflows). The use of Neumann conditions would allow to extend the applicability of the lattice Boltzmann method by prescribing, for example, effects related to $\partial_j u_i$ (e.g. stress over a porous wall, wall models for turbulent flows, hydrophobic-hydrophilic wall treatments) and to reduce the complexity of the domain (e.g. symmetry axis).

In the following, the evolution of the implementation of boundary conditions in lattice Boltzmann methods is reviewed to serve as a basis for the evaluation of the best way to implement Neumann conditions. In this discussion, only macroscopic boundary conditions for the momentum equations are considered. However, the conclusions presented can be extended to any other macroscopic variable.

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The first approach to model walls in LB is the use of the bounce-back scheme (see, for example, [10]) for the non-slip condition, and the application of a specular reflection for the complete slip or zero-stress one. From this straightforward approach it is possible to observe the obvious relationship between the stress at the wall, the wall collision, and the slip condition.

With the bounce-back scheme as the starting point, two pieces of work elaborated on improved boundary conditions for LB. One of them established the influence of the relaxation parameters on the wall location [11] and the other studied the influence of the definition of the non-equilibrium part of the distribution functions on wall (and initial) conditions [12]. Also relevant to the present discussion are some further papers describing alternative approaches to improve the accuracy of the bounce-back boundary condition considering different lattices (e.g. [13–16]).

A first work on including arbitrary geometries was the one by Ginzbourg and d'Humières [17] for a Poiseuille flow in inclined channels. Filippova and Hänel [18] developed an approach for dealing with complex geometries based on modifications to the bounce-back procedure using interpolation; this approach was improved by Mei et al. [19] and [20], and generalized by Ginzburg et al. [21,22]. Another approach to simulate curved geometries is based on the volumetric scheme by Chen et al. [23], that has also been improved upon [24]. The work by Verberg and Ladd [25] can be considered a different way to impose volumetric boundary conditions. One further approach is the extrapolation proposed by Chen et al. [26] and extended to curved geometries by Guo et al. [27]. Two additional concepts have been introduced, related to local boundary conditions [17,28,29], and immersed boundary conditions for lattice Boltzmann methods [30].

The development of Neumann boundary treatments in LB largely focuses on the definition of slip boundaries, or stress-related conditions, as they are linked to the development of wall boundary-conditions for microflows [31–33]. Although the use of kinetic boundary conditions to impose a pre-defined stresses has been attempted for planar walls, no satisfactory result has been obtained in curved geometries, for which their application becomes complex or impossible [32,34].

Some attempts to simulate configurations which need Neumann conditions can be found in the literature [35,34]. The best-suited hydrodynamic approach for setting Neumann conditions at boundaries, even with complex geometries, is often claimed to be the volumetric approach by Chen et al. [23].

The preceding review of boundary conditions for lattice Boltzmann methods provide some guidelines for an efficient implementation of Neumann boundary conditions. Thus, any method proposed should: (i) preserve the simplicity and good stability behavior of bounce-back-based schemes; (ii) be second-order (or higher) for arbitrary geometries; (iii) avoid the use of extrapolations related to hydrodynamic treatments [26]; and (iv) avoid the use of non-lattice distribution functions as in kinetic methods with non-zero off-diagonal kernels [31,36].

The approach presented here treats the problem in a general efficient way preserving well-established boundary treatments [22] and including macroscopic-gradients with a low degree of added complexity. It is a practical approximation to solve the problem that can be formulated in a modular way to introduce improvements that do not change the basic structure.

The paper is organized as follows. Section 2 briefly describes the multi-relaxation-times (MRT) lattice Boltzmann method used to test the boundary treatment proposed. In Section 3 the implementation of gradient-based boundary conditions is introduced. In Section 4 results for different test cases are presented. Finally, (Section 5), some conclusions from the results and an outline of possible applications are discussed.

2. The lattice Boltzmann method

The approach to boundary treatment presented in this paper is independent of the lattice Boltzmann method used. However, we choose an MRT lattice Boltzmann method [37] because the access to a larger number of relaxation factors allows to improve the stability of the method, and to influence the accuracy of the boundary conditions.

A two dimensional (D2Q9) method with nine velocities $\mathbf{e}_i = (e_{x\alpha}, e_{y\alpha})$ with $e_{x\alpha} = (0,1,0,-1,0,1,-1,-1,1)$ and $e_{y\alpha} = (0,0,1,0,-1,1,1,-1,-1)$, is used. The velocity distribution functions $\mathbf{f} \equiv f_\alpha \in \mathbb{R}^9$ evolve according to nine velocities in a two dimensional lattice of nodes $x_i \in \mathbb{Z}^2$. The evolution equation for $\mathbf{f}$ is:

$$\mathbf{f}(x_i + \mathbf{e}_i \delta t, t + \delta t) - \mathbf{f}(x_i, t) = -\mathbf{M}^{-1} \cdot \mathbf{S} \cdot [\mathbf{m}(x_i, t) - \mathbf{m}^{eq}(x_i, t)] \; + \mathbf{F}(x_i, t); \tag{1}$$

where the lower-case-bold symbols, $\mathbf{f}$ and $\mathbf{m}$, denote transpose 9-dimensional vectors; $\mathbf{M}$ is the transformation matrix that linearly relates velocity distribution functions and moments: $\mathbf{f} = \mathbf{M}^{-1} \cdot \mathbf{m}$ and $\mathbf{m} = \mathbf{M} \cdot \mathbf{f}$; $\mathbf{m} = (\rho, e, \epsilon, \rho u_x, q_x, \rho u_y, q_y, p_{xx}, p_{xy})^T$ are the macroscopic moments and $\mathbf{m}^{eq}$ their equilibrium values; $\mathbf{S} = \mathrm{diag}(0, s_e, s_\epsilon, 0, s_\alpha, 0, s_\alpha, s_\nu, s_\nu)$ is a diagonal matrix of relaxation factors, where s_ν is related to the viscosity; c_s is the speed of sound, and $w_\alpha = (4/9, 1/9, 1/9, 1/9, 1/9, 1/36, 1/36, 1/36, 1/36)$ are the weighting coefficients for each velocity. $\mathbf{F} \equiv F_\alpha = 1/c_s^2 w_\alpha \rho_0 \delta t (e_{i\alpha} a_i)$ is an external body force, a_i being the acceleration induced by this force. Additional details about the definition of body forces and their influence on momentum are discussed, for example, in [38]. Further information about the method can be found in the work by Lallemand and Luo [39]. Essentially, we work with a simplified version of the MRT collision operator with only two relaxation times (TRT) [40–43,22,44]. For this case $s_e = s_\epsilon = s_\nu$ and s_α is related to s_ν in order to reduce errors at the boundary in a way which varies depending on the interpolation scheme used. Unless otherwise indicated, we will take $s_\alpha = 8(2 - s_\nu)/(8 - s_\nu)$ [21,22].

Applying a Chapman-Enskog expansion to Eq. (1) the Navier–Stokes equations are recovered in the limit of low Kn and low Ma numbers, with $\rho = \sum_\alpha f_\alpha$ and $\rho u_i = \sum_\alpha (e_{i\alpha} f_\alpha) + F_i/2$. The fluid viscosity is related to s_ν as: $\nu = c_s^2(1/s_\nu - 1/2)$. A speed of sound $c_s = 1/\sqrt{3}$ is considered hereafter.