Asymptotic analysis of extrapolation boundary conditions for LBM

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A B S T R A C T

We present an investigation of extrapolation boundary conditions for lattice Boltzmann method (LBM) using asymptotic analysis. Equilibrium and non-equilibrium extrapolation methods for velocity and pressure boundary conditions proposed in the literature were tested numerically in specific cases. We analyse these boundary conditions using asymptotic expansion techniques and show an improvement in the accuracy of the lattice Boltzmann solution. We also present few numerical examples and simulate fluid flow across an unsymmetrically placed stationary cylinder in a channel with steady and unsteady flow conditions. Thus the article demonstrates application of asymptotic analysis to understand properties of extrapolation boundary conditions for LBM and show the flexibility of these boundary conditions for complex fluid flow applications.

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1. Introduction

Lattice Boltzmann method (LBM) has become an alternative numerical method to solve hydrodynamic problems governed by incompressible Navier–Stokes equations in complex domains. In virtue of its simple formulation, the method can be used to simulate complex fluid flows such as two-phase flows, flow through porous media, electro-hydrodynamics, magneto-hydrodynamics, acoustic streaming etc.

The LBM is based on microscopic models and mesoscopic kinetic equations that model physics of microscopic or mesoscopic processes and averaged macroscopic properties obey desired macroscopic equations. The idea behind LBM using kinetic type methods for macroscopic equations is the fact that, hydrodynamics of the fluid is an effective result of the behaviour of many microscopic particles in the system and the macroscopic dynamics is not sensitive to the underlying microscopic dynamics. The lattice Boltzmann equation can be derived from the classical Boltzmann equation in a discrete velocity space [1].

Asymptotic analysis, a common analysis tool to analyse finite difference equations [2], is an efficient and simple approach to study the relation between the lattice Boltzmann equation (LBE) and the Navier–Stokes equations [3–6]. We restrict the analysis to a diffusive time scale (\(\Delta t = h^2\), \(h\) the space discretization and \(\Delta t\) the time discretization steps) regime as we investigate the relation between the LBE and the incompressible Navier–Stokes equations. The asymptotic analysis is also an effective tool to study the dependence of numerical solution on \(h\) and estimate errors with the exact solution. And asymptotic analysis of LBM [7] in an unbounded domain was shown to result in a second order accuracy in velocity field (\(\mathbf{u}\)) and a first order accuracy in pressure field (\(p\)) for the incompressible Navier–Stokes equations.

In a bounded domain, second order accuracy of the solution for the velocity field can be maintained by defining appropriate boundary conditions. Thus the choice of boundary conditions plays a deciding role in determining accuracy of numerical solution. For example, bounce-back boundary condition is a classical approach to impose no-slip condition on complex boundaries and was shown to be first order accurate in velocity field, except when the boundary is \(h/2\) away from...
the boundary fluid node. A correction to the bounce-back condition is proposed by Bouzidi, Firdaouss and Lallemand (BFL) [8] for arbitrary boundaries and was shown to achieve a second order accuracy in $h$ using asymptotic analysis [9]. Extrapolation boundary conditions proposed in [10,11] are also known to achieve second order accuracy. Investigating the application of asymptotic analysis to these extrapolation boundary conditions is our motivation behind the work presented here.

We briefly outline the contents of the article here. In Section 2, we introduce lattice Boltzmann method, and in Section 3, we discuss briefly about the issues involved in boundary conditions and describe the extrapolation boundary conditions. In Section 4, we describe asymptotic analysis for LBM and show the relation between the lattice Boltzmann equation and the incompressible Navier–Stokes equations. In Section 5, we use the asymptotic analysis tools to analyse the equilibrium extrapolation method for velocity boundary conditions for complex boundaries. And then analyse non-equilibrium extrapolation method for velocity and pressure boundary conditions in the case of flat boundaries. We present numerical examples of Couette flow between two concentric cylinders and a two-dimensional stationary linear flow in a square domain. We show an improvement in the accuracy of the numerical solutions using these extrapolation boundary conditions when compared with bounce-back boundary conditions. We simulate a benchmark laminar flow over an asymmetrically placed cylinder in a channel [12] using extrapolation boundary conditions. We compare drag and lift coefficients with the values reported in literature.

2. The lattice Boltzmann method

LBM is based on a simplified microscopic model of the fluid in which particles travel over a regular spatial lattice $\mathbb{Z}^d$ with constant discrete speed $c_i \in \mathbb{C} = \{c_1, c_2, \ldots, c_m\} \subset \mathbb{Z}^d$, with $j + c_i \in \mathbb{Z}^d$ for each lattice node $j \in \mathbb{Z}^d$. Such a scheme is denoted by DdQM. For example D2Q9 is a two-dimensional scheme with 9 lattice directions and D3Q15 is a three-dimensional scheme with 15 lattice directions.

2.1. Overview

The discretized lattice Boltzmann equation with single relaxation time BGK approximation of the collision operator is given by

$$\hat{f}_i(n + 1, j + c_i) = \hat{f}_i(n, j) - \frac{1}{\tau} \left( \hat{f}_i(n, j) - \hat{f}^{eq}_i(n, j) \right).$$  \hspace{1cm} (1)

Here $\hat{f}_i(n, j)$, components of $\hat{\mathbf{f}} : \mathbb{N} \times \mathbb{Z}^d \rightarrow \mathbb{R}^m$, are particle distribution functions at discrete time $n \in \mathbb{N}$ and at lattice node $j \in \mathbb{Z}^d$ in the direction of $c_i$. $\hat{f}^{eq}_i$ is the equilibrium distribution function. $\tau$ is the time relaxation parameter which is defined by the kinematic viscosity $\nu$ of the fluid as $\tau = \frac{6\nu+1}{2}$.

In this article we consider the D2Q9 setup with 9 lattice directions represented by the columns of the following matrix

$$\mathbf{C} = \begin{pmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{pmatrix}.$$  \hspace{1cm} (2)

For D2Q9, the equilibrium distribution function $\hat{f}^{eq}_i(n, j)$ is defined as

$$\hat{f}^{eq}_i(n, j) \equiv \hat{f}^{eq}_i(\hat{\rho}, \hat{\mathbf{u}}) = f^*_i \left[ \hat{\rho} + 3\hat{\mathbf{c}}_i \cdot \hat{\mathbf{u}} + \frac{9}{2} (\hat{\mathbf{c}}_i \cdot \hat{\mathbf{u}})^2 - \frac{3}{2} \hat{\mathbf{u}} \cdot \hat{\mathbf{u}} \right] (n, j) \hspace{1cm}$$  \hspace{1cm} (2)

where $\hat{\rho}$, $\hat{\mathbf{u}}$ are defined as velocity moments of particle distributions $\hat{f}_i$ given by

$$\hat{\rho} = \sum_i \hat{f}_i$$

$$\hat{\mathbf{u}} = \sum_i \hat{f}_i \hat{\mathbf{c}}_i$$

and $f^*_i$ are constant weights that depend on the domain discretization model. The weights for D2Q9 model are $f^*_i = 4/9$, $f^*_i = 1/9$ for $i = 2, 3, 4, 5$ and $f^*_i = 1/36$ for $i = 6, 7, 8, 9$.

These macroscopic lattice variables approximate the velocity field $\mathbf{u} : [0, T] \times \Omega \rightarrow \mathbb{R}^d$ and the pressure field $p : [0, T] \times \Omega \rightarrow \mathbb{R}$ of the incompressible Navier–Stokes equations

$$\nabla \cdot \mathbf{u} = 0$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} + \nabla p = \nu \nabla^2 \mathbf{u}$$  \hspace{1cm} (3)

on the domain $\Omega \subseteq \mathbb{R}^d$ with appropriate initial and boundary conditions in the absence of external body forces. The lattice nodes $j \in \mathbb{Z}^d$ correspond to the position $\mathbf{x}_i$ in the continuous domain $\Omega$ through the spatial discretization parameter $h > 0$ as $\mathbf{x}_i = jh$. The lattice time $n \in \mathbb{N}$ corresponds to the continuous time $t_n \in [0, T]$ through time discretization parameter $\Delta t > 0$ as $t_n = n\Delta t$. Recalling again, we restrict the analysis to a diffusive time scale regime i.e. $\Delta t = h^2$. 

The lattice Boltzmann evolution equation (1) can be realized in two steps.

Collision:
\[ \hat{f}_i^+(n, j) = \hat{f}_i(n, j) - \frac{1}{\tau} \hat{f}_i^{ne}(n, j). \]  \( (4) \)

Propagation:
\[ \hat{f}_i(n + 1, j + \mathbf{c}_i) = \hat{f}_i^+(n, j). \]  \( (5) \)

Here the non-equilibrium part \( \hat{f}_i^{ne}(n, j) \) of the distribution function is given by
\[ \hat{f}_i^{ne}(n, j) = \hat{f}_i(n, j) - \hat{f}_i^{eq}(n, j). \]

We use the lattice Boltzmann initialization method proposed in [13] to initialize the lattice variables. An asymptotic analysis of initialization algorithms can be found in [14].

3. Lattice Boltzmann boundary conditions

Let \( x_f = x_w + h\mathbf{c}_i \) be a boundary fluid node, where \( x_w \) is a non-fluid node as shown in Fig. 1. Let \( x_b \) be the physical boundary node that intersects the link joining \( x_f \) and \( x_w \), as shown in Fig. 1. Let \( q \in (0, 1] \) be the normalized distance of the boundary node from the fluid node in the incoming direction of \( \mathbf{c}_i \), so that \( x_f = x_b + hq\mathbf{c}_i \) and \( x_w = x_b + h(q - 1)\mathbf{c}_i \).

Observing that, to complete the propagation step (5) at boundary fluid node \( \hat{f}_i(n + 1, \mathbf{f}) \), the collision (4) \( \hat{f}_i^+(n, \mathbf{w}) \) at the wall node has to be computed. Hence, after propagation step, all outgoing populations \( \hat{f}_i^* \) (where \( \mathbf{c}_r = -\mathbf{c}_i \)) at boundary lattice nodes are known. But, the incoming particle distributions \( \hat{f}_i(n + 1, \mathbf{f}) = \hat{f}_i^+(n, \mathbf{w}) \) are unknown as the wall node \( x_w \) is not in the fluid domain. We fill these unknown distributions by defining post collision distributions \( \hat{f}_i^+(n, \mathbf{w}) \) at \( x_w \) to impose boundary conditions. Thus, it is important to note that, lattice Boltzmann boundary conditions are imposed indirectly on the underlying particle distribution function rather than directly on macroscopic variables [15–17].

For example, the classical approach of bounce-back method (6) can be used to impose a no-slip condition on the boundary. In this case, the incoming populations of a boundary fluid node \( x_f \) are defined as
\[ \hat{f}_i^+(n, \mathbf{w}) = \hat{f}_i^+(n, \mathbf{f}) + 6h\hat{f}_i^*\mathbf{c}_i \cdot \mathbf{\phi}(t_n, x_b) \]  \( (6) \)
where \( \mathbf{\phi}(t_n, x_b) \) is the prescribed boundary velocity.

3.1. Extrapolation velocity boundary condition

We define the unknown incoming post collision populations at the wall node using extrapolation methods. The Extrapolation velocity boundary condition is given by
\[ \hat{f}_i^+(n, \mathbf{w}) = \hat{f}_i^{eq}(n, \mathbf{w}) + \left( 1 - \frac{1}{\tau} \right) \hat{f}_i^{ne}(n, \mathbf{w}). \]  \( (7) \)

The density and velocity at the wall node are linearly extrapolated using the value of \( q \), the prescribed boundary velocity \( \mathbf{\phi}(t_n, x_b) \) and the densities of neighbouring fluid nodes as follows. For \( q \geq 0.75 \)
\[ \hat{\rho}_w = \hat{\rho}(n, \mathbf{f}) \]
\[ \hat{\mathbf{u}}_w = \frac{h\mathbf{\phi} + (q - 1)\hat{\mathbf{u}}_f}{q} \]  \( (8) \)
\[ \hat{f}_i^{ne}(n, \mathbf{w}) = \hat{f}_i^{ne}(n, \mathbf{f}) \]
and for \( q < 0.75 \)
\[ \hat{\rho}_w = \hat{\rho}(n, f) \]
\[ \hat{u}_w = h\phi + (q - 1)\hat{u}_t + \frac{1 - q}{1 + q} (2h\phi + (q - 1)\hat{u}_n) \]
\[ \hat{f}^{ne}_i(n, w) = \hat{q}^{ne}_i(n, f) + (1 - q)\hat{f}^{ne}_i(n, ff). \]

Here the subscripts \( f \) and \( ff \) denote the quantities at \( x_f \) and \( x_{ff} \) respectively as shown in Fig. 1.

3.2. Non-equilibrium extrapolation boundary conditions

The non-equilibrium extrapolation for velocity and pressure boundary conditions is defined only for flat boundaries with \( q = 1 \). The non-equilibrium extrapolation for velocity boundary condition is equivalent to the above described extrapolation velocity condition for arbitrary boundaries with \( q = 1 \). Hence we analyse here only the non-equilibrium extrapolation method for pressure condition for flat boundaries. We define the unknown post collision populations at the wall node as follows

\[ \hat{f}^+_i(n, w) = \hat{f}^{eq}_i(1 + 3h^2\phi(t_n, x_b), \hat{u}_f) + \left( 1 - \frac{1}{r} \right) \hat{f}^{ne}_i(n, f) \]

where \( \phi(t_n, x_b) \) is the prescribed pressure on the boundary.

4. Asymptotic analysis

In this section we briefly describe the asymptotic analysis of LBM introduced in [7]. Asymptotic analysis is an efficient approach to study the dependence of lattice variables \( \hat{\rho} \) and \( \hat{u} \) on a small discretization parameter \( h > 0 \). We can also determine the order of accuracy of numerical solution to the incompressible Navier–Stokes pressure \( \rho \) and velocity \( u \). Consider the following asymptotic expansion with continuous coefficients of lattice macroscopic variables

\[ \hat{\rho}(n, j) = \rho^{(0)}(t_n, x_j) + h^2\rho^{(2)}(t_n, x_j) + \cdots \]
\[ \hat{u}(n, j) = h\hat{u}^{(1)}(t_n, x_j) + h^2\hat{u}^{(2)}(t_n, x_j) + \cdots. \]

In general, we can express the particle distributions as a series expansion shown below

\[ \hat{f}_i(n, j) = f_i^{(0)}(t_n, x_j) + h f_i^{(1)}(t_n, x_j) + h^2 f_i^{(2)}(t_n, x_j) + \cdots \]

with \( f_i^{(0)} = f_i^* \) and \( f_i^{(m)} \) are \( h \)-independent smooth functions. \( \rho^{(m)}, u^{(m)} \) are defined as

\[ \rho^{(m)}(t_n, x_j) = \sum_i f_i^{(m)}(t_n, x_j) \]
\[ u^{(m)}(t_n, x_j) = \sum_i f_i^{(m)}(t_n, x_j)c_i. \]

A similar series expansion of the equilibrium (2) and non-equilibrium distribution functions takes the following form

\[ \hat{f}^{eq}_i(n, x_j) = f_i^{eq,(0)} + h f_i^{eq,(1)} + h^2 f_i^{eq,(2)} + \cdots \]
\[ \hat{f}^{ne}_i(n, x_j) = f_i^{ne,(0)} + h f_i^{ne,(1)} + h^2 f_i^{ne,(2)} + \cdots \]

where

\[ f_i^{eq,(m)} = f_i^* + 3c_iu^{(m)} + \frac{9}{2} \left[ \sum_{k+m} \left( \langle c_i, u^{(k)} \rangle (c_i, u^{(l)}) - \frac{1}{3} (u^{(k)}, u^{(l)}) \right) \right] f_i^{ne,(m)} \]

Using the assumption of diffusive scaling, \( (\Delta t = h^2) \) and the smoothness of coefficients \( f_i^{(k)} \), the term \( f_i^{(k)}(t_n + h^2, x_j + hc_i) \) can be expanded around \( (t_n, x_j) \) using the Taylor series

\[ f_i^{(k)}(t_n + h^2, x_j + hc_i) = f_i^{(k)} + h c_i \cdot \nabla f_i^{(k)} + h^2 \left( \frac{\partial}{\partial t} + \frac{(c_i \cdot \nabla)^2}{2} \right) f_i^{(k)} \]
\[ + h^3 (c_i \cdot \nabla)^3 \left( \frac{\partial}{\partial t} + \frac{(c_i \cdot \nabla)^2}{6} \right) f_i^{(k)} + \cdots. \]

Using the above asymptotic expansions (11)–(15), Taylor series expansion (16) in the lattice Boltzmann equation (1) and comparing the coefficients in the order of \( h \) on either side of the equation, we obtain the following relations on the continuous
Using the above expansions of \( f_i^{(k)} \) have for

\[
\begin{align*}
\hat{h}^0 & : f_i^{(0)} = f_i^{eq,(0)} = f_i^* \rho^{(0)} \\
\hat{h}^1 : f_i^{(1)} = f_i^{eq,(1)} = 3f_i^* c_i u^{(1)} \\
\hat{h}^2 : f_i^{(2)} = f_i^{eq,(2)} - \tau (c_i \cdot \nabla) f_i^{(1)} \\
\hat{h}^3 : f_i^{(3)} = f_i^{eq,(3)} - \tau \left( (c_i \cdot \nabla) f_i^{(2)} + \left( \frac{\partial}{\partial t} + \frac{(c_i \cdot \nabla)^2}{2} \right) f_i^{(1)} \right).
\end{align*}
\]

(17)

The above relations are true in the interior of domain \( \Omega \) for each velocity direction \( c_i \). Taking the velocity moments of the relations (17), we obtain the following equations

\[
\nabla \cdot \mathbf{u}^{(1)} = 0
\]

\[
\frac{\partial \mathbf{u}^{(1)}}{\partial t} + (\mathbf{u}^{(1)} \cdot \nabla) \mathbf{u}^{(1)} + \frac{\nabla \rho^{(2)}}{3} = \nu \Delta \mathbf{u}^{(1)}.
\]

(18)

We observe from (18) that \( \mathbf{u}^{(1)} \) is a solution of incompressible Navier–Stokes equation (3) with \( \rho^{(2)}/3 \) the corresponding kinematic pressure. Continuing the analysis to other orders of \( h \), we also observe that \( \mathbf{u}^{(2)} = 0 \). This implies that the Navier–Stokes velocity \( \mathbf{u} = \mathbf{u}^{(1)} = \hat{u}/h + o(h^2) \), is second order accurate velocity field in \( h \), and the Navier–Stokes pressure \( p = \rho^{(2)}/3 = (\hat{\rho} - \rho^{(0)})/3h^2 + o(h) \), is first order accurate. Since \( \rho^{(0)} = \sum_i f_i^{(0)} = \sum_i f_i^* = 1 \) we have

\[
\rho^{(2)}/3 = (\hat{\rho} - 1)/3h^2 + o(h).
\]

5. Asymptotic analysis of extrapolation boundary conditions

In this section, we apply the asymptotic analysis to the extrapolation velocity boundary conditions and non-equilibrium extrapolation for pressure boundary conditions. In the first subsection, we analyse the extrapolation velocity conditions for a general geometry \( g \) and deduce that \( \mathbf{u}^{(2)} = 0 \) i.e. second order accurate in \( h \). And in the following subsection, we analyse the non-equilibrium extrapolation for pressure boundary conditions and show that it is an alternative way to impose pressure conditions that does not reduce the accuracy in pressure.

5.1. Asymptotic analysis of extrapolation method for velocity boundary conditions

Assuming the following series expansions approximate the macroscopic variables at the boundary fluid node

\[
\hat{u}(n, \mathbf{f}) = h\mathbf{u}^{(1)}(t_n, \mathbf{x}_t) + h^2\mathbf{u}^{(2)}(t_n, \mathbf{x}_t) + \cdots
\]

\[
\hat{\rho}(n, \mathbf{f}) = \hat{\rho}(t_n, \mathbf{f}) = 1 + h^2\rho^{(2)}(t_n, \mathbf{x}_b) + \cdots.
\]

Expanding the coefficients in a Taylor series around the boundary node \( (t_n, \mathbf{x}_b) \), using the fact that \( \mathbf{x}_t = \mathbf{x}_b + qh\mathbf{c}_i \) and \( \mathbf{x}_f = \mathbf{x}_b + (1 + q)qh\mathbf{c}_i \), we obtain

\[
\hat{u}(n, \mathbf{f}) = h\mathbf{u}^{(1)}(t_n, \mathbf{x}_b) + h^2 \left( \mathbf{u}^{(2)}(t_n, \mathbf{x}_b) + q(c_i \cdot \nabla)\mathbf{u}^{(1)}(t_n, \mathbf{x}_b) \right) + \cdots
\]

\[
\hat{u}(n, \mathbf{f}) = h\mathbf{u}^{(1)}(t_n, \mathbf{x}_b) + h^2 \left( \mathbf{u}^{(2)}(t_n, \mathbf{x}_b) + (1 + q)c_i \cdot \nabla\mathbf{u}^{(1)}(t_n, \mathbf{x}_b) \right) + \cdots
\]

\[
\hat{\rho}(n, \mathbf{f}) = \hat{\rho}(t_n, \mathbf{f}) = 1 + h^2\rho^{(2)}(t_n, \mathbf{x}_b) + \cdots.
\]

Substituting the above expansions into \( \hat{\mathbf{u}}_w \) in (8) and (9) assuming the form \( \hat{\mathbf{u}}_w = h\mathbf{a}(t_n, \mathbf{x}_b) + h^2\mathbf{b}(t_n, \mathbf{x}_b) + \cdots \) then we have for \( q \geq 0.75 \)

\[
\mathbf{a}(t_n, \mathbf{x}_b) = \frac{1}{q} \phi(t_n, \mathbf{x}_b) + \left( \frac{q - 1}{q} \right) \mathbf{u}^{(1)}(t_n, \mathbf{x}_b)
\]

\[
\mathbf{b}(t_n, \mathbf{x}_b) = \left( \frac{q - 1}{q} \right) \mathbf{u}^{(2)}(t_n, \mathbf{x}_b) + (q - 1)(c_i \cdot \nabla)\mathbf{u}^{(1)}(t_n, \mathbf{x}_b)
\]

(19)

and for \( q < 0.75 \)

\[
\mathbf{a}(t_n, \mathbf{x}_b) = \left( \frac{3 - q}{1 + q} \right) \phi(t_n, \mathbf{x}_b) + 2 \left( \frac{q - 1}{1 + q} \right) \mathbf{u}^{(1)}(t_n, \mathbf{x}_b)
\]

\[
\mathbf{b}(t_n, \mathbf{x}_b) = 2 \left( \frac{q - 1}{1 + q} \right) \mathbf{u}^{(2)}(t_n, \mathbf{x}_b) + (q - 1)(c_i \cdot \nabla)\mathbf{u}^{(1)}(t_n, \mathbf{x}_b).
\]

(20)

Using the above expansions of \( \hat{\rho}_w \) and \( \hat{\mathbf{u}}_w \) around the boundary node \( \mathbf{x}_b \), the equilibrium distribution function at the wall node \( \mathbf{x}_w \) in (7) take the following form

\[
\hat{g}_{f_i}^{eq}(\hat{\rho}_w, \hat{\mathbf{u}}_w) = f_i^* \left( 1 + 3hc_i \cdot \mathbf{a} + h^2 \left( \rho^{(2)} + 3c_i \cdot \mathbf{b} + \frac{9}{2}(c_i \cdot \mathbf{a})^2 - \frac{3}{2}c_i \cdot \mathbf{a} \right) \right) + \cdots.
\]

(21)
Also in both the cases (8) and (9), the non-equilibrium part can be expanded as

\[ \hat{f}^\text{ne}(n, \mathbf{w}) = h^2 \hat{f}^\text{ne,}(2) (t_n, \mathbf{x}_b) + \cdots \]

Expanding the propagation step (5) in a Taylor series around the boundary node \( \mathbf{x}_b \), we have

\[ \hat{f}_i(n + 1, \mathbf{f}) = f_i(n, \mathbf{f}) + h \left( f_i^{(1)} + q (\mathbf{c}_i \cdot \nabla) f_i^{(0)} \right) + h^2 \left[ f_i^{(2)} + q (\mathbf{c}_i \cdot \nabla) f_i^{(1)} \right] \]

\[ + \left( \frac{\partial}{\partial t} + q \frac{1}{2} (\mathbf{c}_i \cdot \nabla)^2 \right) f_i^{(0)} + \cdots. \]  

Comparing the coefficients in order of \( h \) using the relations in (17), we get

\[ h^0 : f_i^{(0)} (t_n, \mathbf{x}_b) = f_i^* \]

\[ h^1 : f_i^{(1)} (t_n, \mathbf{x}_b) = 3f_i^* \mathbf{c}_i \cdot \mathbf{a}(t_n, \mathbf{x}_b) \]

i.e.

\[ 3f_i^* \mathbf{c}_i \cdot \left( \mathbf{u}^{(1)} (t_n, \mathbf{x}_b) - \mathbf{a}(t_n, \mathbf{x}_b) \right) = 0. \]  

Comparing the coefficients for \( h^2 \), we find

\[ f_i^{(2)} + q (\mathbf{c}_i \cdot \nabla) f_i^{(1)} = f_i^* \left( \rho^{(2)} + 3 \mathbf{c}_i \cdot \mathbf{b} + \frac{9}{2} (\mathbf{c}_i \cdot \mathbf{a})^2 - \frac{3}{2} \mathbf{a} \cdot \mathbf{a} \right) + \left( 1 - \frac{1}{\tau} \right) f_i^{\text{ne,}(2)} \]

which implies that

\[ 3f_i^* \mathbf{c}_i \cdot \left( \mathbf{u}^{(2)} (t_n, \mathbf{x}_b) - \mathbf{b}(t_n, \mathbf{x}_b) + (q - 1) (\mathbf{c}_i \cdot \nabla) \mathbf{u}^{(1)} (t_n, \mathbf{x}_b) \right) = 0. \]  

Using the expression for \( \mathbf{b}(t_n, \mathbf{x}_b) \) in (24), we can deduce the condition

\[ \mathbf{u}^{(2)} (t_n, \mathbf{x}_b) = 0. \]

All the above conclusions are true since there are at least two (D2Q9) linearly independent incoming directions at a boundary node. Hence

\[ \mathbf{u}^{(1)} = \hat{\mathbf{u}} / h + O(h^2) \]

and the analysis demonstrates that the velocity field is second order accurate.

5.2. Asymptotic analysis of non-equilibrium extrapolation method for pressure boundary conditions

The algorithm for the non-equilibrium extrapolation method for pressure boundary conditions is given by

\[ \hat{f}_i^+ (n, \mathbf{w}) = \hat{f}_i^0 (1 + 3h^2 \phi(t_n, \mathbf{x}_b), \hat{\mathbf{u}}_f) + \left( 1 - \frac{1}{\tau} \right) \hat{f}_i^{\text{ne}} (n, \mathbf{f}) \]  

where \( \phi(t_n, \mathbf{x}_b) \) is the prescribed pressure on the boundary. We observe that this can be rewritten as follows

\[ \hat{f}_i^+ (n, \mathbf{f}) = \hat{f}_i^0 (n, \mathbf{f}) - \frac{1}{\tau} \hat{f}_i^{\text{ne}} (n, \mathbf{f}) + f_i^* \left( 1 + 3h^2 \phi(t_n, \mathbf{x}_b) - \hat{\rho}(n, \mathbf{f}) \right). \]

Using the asymptotic and Taylor series expansions around the boundary node \( \mathbf{x}_b \) in the above equation, we have

\[ \hat{f}_i^+ (n, \mathbf{f}) = f_i^{(0)} + h f_i^{(1)} + h^2 \left( f_i^{(2)} - \frac{1}{\tau} f_i^{\text{ne,}(2)} + f_i^* (3 \phi - \rho^{(2)}) \right). \]  

Now comparing the coefficients of \( h^2 \) of (22) and (26), either side of propagation step (5) we find

\[ f_i^{(2)} + (\mathbf{c}_i \cdot \nabla) f_i^{(1)} = f_i^{(2)} - \frac{1}{\tau} f_i^{\text{ne,}(2)} + f_i^* (3 \phi - \rho^{(2)}) \]

which implies that

\[ \frac{\rho^{(2)}}{3} = \phi(t_n, \mathbf{x}_b). \]

Hence,

\[ \phi(t_n, \mathbf{x}_b) = (\hat{\rho} - 1) / 3h^2 + O(h), \]

which shows that the pressure is of first order accurate.
6. Numerical results

In this section, we present few numerical examples that illustrate second order accuracy of extrapolation methods for velocity boundary conditions. In Section 6.1 we present a Couette flow between two concentric circular cylinders and in Section 6.2 a stationary linear flow in a rotated square domain to study the convergence with respect to the space discretization parameter \( h \). Finally in Section 6.3, we perform a benchmark simulation of a steady and unsteady flow over an asymmetrically placed cylinder in a long channel. We use extrapolation boundary conditions on the walls and surface of cylinder. We then compute the drag and lift forces acting on the cylinder and measure the pressure difference between the two ends of the cylinder in the case of steady flow. In addition to these parameters, in the case of unsteady flow, we also measure the Strouhal number that defines the frequency of the Karman vortices that were induced in the wake of the cylinder. We compare these parameters with the values given in literature.

6.1. Couette flow between two concentric circular cylinders

We consider a Couette flow between two concentric circular cylinders where the inner cylinder of radius \( r_1 \) rotates with constant angular velocity \( \omega \) about its axis and the outer cylinder with radius \( r_2 \) is static. We use extrapolation methods on the surfaces of these cylinders for the velocity boundary conditions. Such a Couette flow has the following analytic solution [10]

\[
    u_e(r, \theta) = \frac{u_0 \beta}{1 - \beta^2} \left( \frac{r_2}{r} - \frac{r}{r_2} \right)
\]

where \( u_0 = \omega r_1 \) and \( \beta = r_1/r_2 \). The Reynolds number of the flow is defined as \( Re = (r_2 - r_1)u_0/\nu \). For the convergence studies in this case, we used \( \tau = 0.6 \) and \( \beta = 0.5 \). We simulate the flow at \( Re = 5 \) and \( 20 \) with \( r_1 = 8, 16 \) and \( 32 \). A log plot of the relative global error \( E \) in the velocity field is shown in Fig. 2, and the slope of the curve confirms a second order convergence.

\[
    E = \frac{\|u_e - \hat{u}\|_2}{\|u_e\|_2}
\]

where \( u_e \) is the exact solution and \( \hat{u} = |\hat{u}| \) is the LBM solution.

6.2. Two-dimensional stationary linear flow

The non-local nature of extrapolation boundary conditions is a shortcoming in the case of imposing boundary condition at lattice nodes for which the necessary fluid boundary nodes does not exist. For example, corner nodes of a square geometry. In practice, the bounce-back condition is applied to such lattice nodes but this results in a reduction of the accuracy of the solution in the whole domain. The one-point boundary condition, a correction to classical bounce-back rule, proposed by Junk et al. [18] in conjunction with Bouzidi boundary condition was shown to overcome the problem. In this subsection, we consider a two-dimensional stationary linear flow in a rotated unit square \( \left( \frac{-1}{2}, \frac{1}{2} \right)^2 \) by an angle of 45°. We use extrapolation velocity boundary conditions on the walls and combine the extrapolation boundary condition with the one-point boundary.
correction at the corner nodes to show the second order accuracy of extrapolation condition. We start the lattice Boltzmann
evolution with the exact solution for the stationary flow

$$u(x) = Ax, \quad p(x) = -\frac{1}{2}x^T A^2 x, \quad A = \begin{pmatrix} 4 & 1 \\ 1 & -4 \end{pmatrix}.$$  

The grid sizes considered for the convergence study here are $h = \frac{1}{10}, \frac{1}{20}, \frac{1}{30}, \frac{1}{40}, \frac{1}{50}$ and the viscosity $\nu = 0.1$ with $T = 1$. The lattice Boltzmann solution for velocity and pressure fields are shown in Fig. 3(a), (b). It was observed that the error is inconsistent when the corner nodes were treated by bounce-back condition with an order of accuracy of 1.4901. And when the corner nodes were treated by one-point condition we observe an improvement in order of accuracy to 2.0541 in velocity field as shown in Fig. 3(c). This clearly shows the second order convergence in velocity field and the necessity for special treatment of corner nodes.

6.3. Benchmark geometry

Flow past a circular cylinder is a classical two-dimensional problem for which a large number of experimental and numerical results are available. We consider two-dimensional benchmark test case of flow around a static cylinder, specified in [12] as shown in Fig. 4.

The kinematic viscosity of the fluid is specified to be $\nu = 10^{-3} \text{m}^2/\text{s}$ and fluid density $\rho = 1.0 \text{ kg/m}^3$. $H = 0.41 \text{ m}$ is height of the channel and $D = 0.1$ is diameter of the cylinder. We specify the following parabolic inflow boundary condition

$$u_x(0, y) = 4U_\infty y (H - y)/H^2, \quad u_y = 0, \quad u_z = 0$$
The Reynolds number is defined by $Re = \overline{U}D/\nu$ with mean velocity $\overline{U} = 2u_x(0,H/2)/3$. The drag and lift coefficients are respectively given by

$$C_d = \frac{2F_x}{\rho U^2 D}$$

$$C_l = \frac{2F_y}{\rho U^2 D}$$

$F_x, F_y$ are $x$ and $y$ components of the force $\mathbf{F}$ with flow direction in $x$.

We carry out series of computations to see the convergence of solution with $h$ to the experiment values reported in literature. We discretize the domain with $h = 1/100$ m, 1/200 m, 1/300 m and simulate the flow for several Mach numbers (Ma). We use extrapolation methods to impose boundary conditions on the surface of the cylinder, the inlet and the walls of channel. A homogenous Neumann condition is applied at the outflow. The force components are computed using the momentum exchange method proposed in [20].

### 6.3.1. Steady flow around cylinder

In the case of steady flow, $U_m = 0.3$ m/s for which the Reynolds number is $Re = 20$. Drag coefficient $C_d$, lift coefficient $C_l$ and pressure difference $\Delta P$ are the quantities that we computed in this case. The lattice Boltzmann velocity and pressure fields for the steady laminar flow are shown in Fig. 5(a), (b). The results for steady flow around cylinder are tabulated in Table 1 and clearly demonstrate the convergence of computed quantities to the reference values with finer discretization.

### 6.3.2. Unsteady flow around cylinder

In the case of unsteady flow around a cylinder, $U_m = 1.5$ m/s for which the Reynolds number is $Re = 100$. We compute maximum drag coefficient $C_d$, lift coefficient $C_l$ and pressure difference $\Delta P$ as functions of time for one period [$t_0, t_0 + 1/f$] where $f$ is the characteristic frequency of vortex shedding. $f$ is determined by using Fast Fourier Transform (FFT) of time
Fig. 6. (a) Velocity and (b) pressure field for unsteady flow around cylinder.

Table 2

Results in the case of unsteady flow.

<table>
<thead>
<tr>
<th></th>
<th>$h = \frac{1}{100}$ m</th>
<th>$h = \frac{1}{200}$ m</th>
<th>$h = \frac{1}{300}$ m</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lift coefficient</td>
<td>1.6015</td>
<td>1.0787</td>
<td>0.9937</td>
<td>0.9990–1.0100</td>
</tr>
<tr>
<td>Pressure difference</td>
<td>2.9604</td>
<td>2.7318</td>
<td>2.5051</td>
<td>2.4800–2.500</td>
</tr>
<tr>
<td>Strouhal number</td>
<td>0.2875</td>
<td>0.3000</td>
<td>0.3000</td>
<td>0.2950–0.3050</td>
</tr>
</tbody>
</table>

series of C and is used to compute Strouhal number $St = \frac{Df}{\bar{U}}$. The lattice Boltzmann velocity and pressure fields for the unsteady laminar flow are shown in Fig. 6(a), (b) and Von Karman vortices are clearly visible in the wake of the cylinder. The results for unsteady flow around the cylinder are tabulated in Table 2 and demonstrate the convergence of computed quantities to the reference values with finer discretization.

7. Summary and conclusions

The accuracy of extrapolation and non-equilibrium extrapolation boundary conditions for LBM are investigated using asymptotic analysis. We have shown that extrapolation velocity boundary condition for arbitrary boundaries results in second order accuracy. And non-equilibrium extrapolation pressure boundary condition for flat boundaries results in first order accuracy for the Navier–Stokes pressure field. The example of Couette flow between two circular cylinders confirmed the second order accuracy of the extrapolation velocity boundary condition. We have shown an improvement from first order when the bounce-back condition is used. The non-local nature of the extrapolation condition was a disadvantage whenever necessary boundary fluid nodes were not present. But with the example of linear stationary flow in rotated square domain, we have shown to overcome by using the one-point boundary condition correction to the incoming populations at corner nodes. Finally, we set up a steady and unsteady channel flow around a circular cylinder with benchmark flow conditions specified in [12]. We have shown that the numerical results are in good agreement with and converge to the experimental results reported in literature.

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